Studentská odborná konference
Chemie je život 2019

Sborník abstraktů

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Sborník abstraktů

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Obsah

Sekce středoškolských studentů

Sekce studentů bakalářských a magisterských studijních programů

Sekce studentů doktorských studijních programů Tématický okruh organická, enviromentální a biochemie

Sekce studentů doktorských studijních programů
Tématický okruh anorganická chemie, materiálové vědy a inženýrství

Sekce středoškolských studentů

Význam a způsoby měření extrakorpuskulárního hemoglobinu v krevní plazmě

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Cílem práce je určit rychlou, levnou a lehce dostupnou metodu pro stanovení extrakorpuskulárního (volného) hemoglobinu v krevní plazmě. Jedná se o metodu dle Fairbankse, jež je založena na měření absorbance plazmy pomocí spektrofotometru. Naměřená absorbance se následně dosadí do stanovené výpočtové metody.

Červené krvinky (erytrocyty) obsahují červené krevní barvivo hemoglobin. Pokud dojde k rozpadu červených krvinek, odborně se tento proces označuje jako hemolýza, hemoglobin se uvolní do plazmy. Nejčastěji je hemolýza způsobena chemickými či fyzikálními vlivy, například při změně vnitřního prostředí, dále při užívaní léků, především antibiotik nebo při styku s toxickými látkami, mezi které patří například olovo. V plazmě je hemoglobin vychytáván plazmatickým glykoproteinem haptoglobinem, a vzniká tak komplex haptoglobin-hemoglobin. Pokud se mezi nimi vysytí vazebná kapacita, vzniká extrakorpuskulární hemoglobin, který je v plazmě škodlivý.

V práci se zaměřuji na měření koncentrace volného hemoglobinu jak u zdravých lidí, tak u pacientů s různým onemocněním. Nejzávažnější onemocnění, se kterým jsem se během práce setkala, byl pacient se srdečním selháním. Pacient byl připojen na extrakorporální membránovou oxygenaci (ECMO). ECMO je uznávaná záchranná metoda mechanické podpory v oběhu, která umožňuje dočasně nahradit právě srdeční selhání či funkci plic.

Klíčová slova: absorbance, centrifugace, extrakorpuskulární hemoglobin, plazma, spektrofotometrie, vlnová délka

Vliv mikrovlnného ohřevu na uvolňování esterů kyseliny ftalové z potravinových plastů

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Tato práce se zaměřuje na diestery kyseliny ftalové (ftaláty), konkrétně di(2--ethylhexyl)-ftalát (DEHP) a dibutyl-ftalát (DBP). Rozebírá jejich vlastnosti, využití a vliv na organismy. Ftaláty jsou používány především jako změkčovadla plastických hmot. S polymery však nijak chemicky nereagují a nejsou v nich pevně vázány. Z tohoto důvodu se uvolňují do životního prostředí a kumulují se v živočiších. Praktická část studuje migraci ftalátů z plastových misek do simulantů potravin vlivem mikrovlnného ohřevu.

Přímá elektrochemická detekce bílkovin a jejich komplexů na nabitých površích

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V naší práci se zabýváme chováním bílkoviny BSA a jejími složkami – monomery a dimery na nabitých površích (elektrodách). Hlavní metodou měření je chronopotenciometrie, díky které lze změřit různé závislosti, například na koncentraci, proudu, potenciálu nebo čase. K výzkumu jsme využily i dalších elektrochemických metod jako je UV spektrofotometrie nebo elektroforéza. Cílem práce je zjistit, jaké jsou rozdíly v chování monomeru a dimeru BSA.

Klíčová slova: BSA, bovine serum albumin, protein, rtuťová elektroda, stříbrná elektroda, koncentrace, proud, potenciál, fosfátový pufr, chronopotenciometrie

Laserová fotoakustická spektroskopie

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Práce se zabývá laserovou fotoakustickou spektroskopií, metodou založenou na tvorbě akustických vln v uzavřené kyvetě se zkoumaným plynem, které jsou pak snímány špičkovým kondenzátorovým mikrofonem a optickým mikrofonem, pro jehož základ byla v této práci požita tenká slídová membrána (cantilever). Díky tomuto dvojitému detekčnímu systému patří laserová fotoakustická spektroskopie mezi velmi citlivé, a ne příliš drahé metody, které jsou vhodné pro kvantitativní a kvalitativní analýzu plynů s nízkou koncentrací. Kromě představení principu a měřící soustavy LFS je pomocí koncentračního měření s N_2O porovnána citlivost cantileveru s citlivostí kondenzátorového mikrofonu. Z výsledků lze určit vhodnost použití cantileveru při laserové fotoakustické spektroskopii. Metoda je mimo jiné vhodná například při kontrole anestezie, pro pracovní hygienu a obecně pro kontrolu plynů enviromentálních emisí.

Klíčová slova: fotoakustická spektroskopie, cantilever, laser, mikrofon

Charakter vod a půd na antropogenních odvalech po těžbě polymetalických rud

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Cílem naší práce je výzkum vod vytékajících ze středověkých štol Cumberk a Utín a posouzení, zda jejich vlivem nedochází k okyselování prostředí na antropogenních haldách.

Štola Cumberk se nachází u obce Švařec u Štěpánova nad Svratkou. Těžilo se zde hlavně stříbro. Areál těžby se rozprostírá na 22 hektarech. Námi studovaná důlní voda byla měřena na třech místech – přímo u výtoku ze štoly, cca 5 metrů pod výtokem ze štoly a cca 5 metrů nad výtokem ze štoly ve spodní části areálu, kde nad Záskalským potokem je dnes z velké části zasypána pravděpodobná štola, která sloužila na odvodnění důlních děl.

Další námi pozorovaná štola spadá do katastru obce Utín u Přibyslavi. Jedná se o jeden z nejstarších doložených těžebních areálů v ČR. Zrudnění na této lokalitě je tvořeno minerály arzenopyritem, pyritem, sfaleritem a galenitem, těžilo se však zde převážně stříbro. Na této lokalitě jsme vodu měřily pouze na jednom místě, a to přímo ve výtoku ze štoly.

Na obou lokalitách jsme odebraly vzorky hlíny. Na Utíně 3 vzorky a na Cumberku 6 z důvodu větší rozlehlosti areálu. V laboratoři jsme z nich vytvořily výluhy v ředění 1:5 a 1:10 a pomocí multimetru jsme měřily pH a vodivost těchto vzorků. Z naměřených výsledků posuzujeme, zda voda ovlivňuje kyselost půdy na lokalitách.

Fluorescenční in situ hybridizace Y specifických repetitivních sekvencí u dioetického druhu šťovíku kyselého

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Tato práce je založena na zkoumání Y chromozomu rostliny šťovíku kyselého (*Rumex acetosa*). Hlavním cílem práce je zkoumání určitých sekvencí na Y chromozomech, které nám mají pomoci zjistit původ a vznik těchto Y chromozomů. Podrobné informace o struktuře a sekvencích Y chromozomů jsou získávány prostřednictvím fluorescenční mikroskopie, kde je využito schopností chromozomu se barvit.

Osmolarita parenterálních přípravků

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Parenterální léčiva jsou sterilní lékové formy, které neprochází zažívacím traktem. Jedná se zejména o injekce, infuze či implantáty. Lidské tělo si pomocí speciálních regulačních mechanismů udržuje stálou hodnotu homeostáze rovnováha je přímo ovlivněna osmotickým tlakem. Proto je důležité, aby parenterální přípravky, zvláště infuze, byly z hlediska osmotického tlaku shodné s tělesnými tekutinami a nevyvolávaly nadměrný přestup vody z důvodu velkých rozdílů koncentrace. K přesnějšímu popisu míry osmotických vlivů roztoku po aplikaci do organismu se používá vyjádření pomocí osmotické koncentrace v osmolech, tj. osmolalita m_{os} (mOsmol/kg) a osmolarita c_{os} (mOsmol/l). Rozdíl mezi těmito dvěma pojmy je, že osmolalita je prakticky naměřená a převádí se na kilogramy a osmolarita je vypočítaná a převádí se na litry. Tyto termíny bývají často zaměňovány zdravotnickými a laboratorními pracovníky i v odborné literatuře. Práce se zabývá neshodou těchto dvou hodnot.

Experimentální měření prachových částic ve vnitřním a vnějším prostředí Ústavu mikrobiologie PřF MU

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Tato středoškolská odborná činnost na téma „Experimentální měření prachových částic ve vnitřním a vnějším prostředí Ústavu mikrobiologie PřF MU“ se zabývá měřením počtu prachových částic o různých velikostních jednotkách ve vnitřním a vnějším prostředí MUNI. Cílem naší práce bylo zjistit, jaké množství prachových částic obsahuje kancelář, laboratoř a vnější okolí Masarykovy univerzity v Brně. Dále bylo naším cílem zjistit aktuální normy a vyhlášky vztahující se k dané problematice, a zda naše výsledky odpovídají předepsaným normám.

Klíčová slova: oxid uhličitý, teplota, mikroklima, ovzduší, vzduchotechnika, prach

Účinnost mýdla a dezinfekčních prostředků na mikrofloru pokožky ruky

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Cílem této práce bylo zjistit a porovnat účinnost vybraných přípravků určených k hygieně a dezinfekci rukou. I když kůže představuje vysoce účinnou bariéru vůči pronikání mikrobů, tak ruce můžeme považovat za jednu ze vstupních bran onemocnění. Ruce se mohou kontaminovat prostřednictvím kontaktů s různými místy či předměty. Proto jsme vybraly přípravky běžně dostupné v drogerii nebo lékárně. A také používané veřejností. Chtěly jsme zjistit který přípravek je aktericidně nejúčinnější.

Klíčová slova: hygiena rukou, prevence, otisková metoda, hrubé nečistoty, mikroorganismy

Je opravdu potřeba hnojit? Aneb využití chemie v praxi.

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Práce je zaměřena na využití chemie v praxi, respektive na využití chemické metodiky při potřebě hnojení půdy. Středoškolská odborná činnost se zabývá stanovením Agrochemického zkoušení zemědělských půd. V naší práci se zabýváme konkrétně hnojícími přípravky a jejich vliv na půdu. Cílem práce bylo stanovení obsahů vybraných makroprvků (Ca, Mg, K, P, N) v půdě a měření výměnné kapacity půdy na vybrané lokalitě. Výsledky stanovení makroprvků a měření výměnné kapacity nám měly ukázat, zda je opravdu potřeba hnojit či nikoliv. Stanovení makroprvků vápníku, hořčíku a draslíku bylo provedeno pomocí atomové absorpční spektrometrie. Fosfor byl stanovován metodou molekulové absorpční spektrofotometrie. Metodou dle Kjeldahla byl stanoven dusík. Půdní reakce neboli pH byla stanovena potenciometricky.

Klíčová slova: úrodnost půdy, makroprvky

Interakce peptidů s modelovými buněčnými membránami

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Moje středoškolská odborná činnost se zaměřuje na jeden z aktuálních problémů ve zdravotnictví. A tím, je rostoucí počet bakterií rezistentních na antibiotika. Hledají se různá řešení, která by mohla antibiotika nahradit. Nadějnou alternativou jsou právě antimikrobiální peptidy, jejichž schopností je cíleně poškodit membránu bakterií vytvořením póru a tím bakterie účinně zabíjet.

Ve své práci se zabývám působením antimikrobiálního peptidu na modely buněčných membrán. Konkrétně synteticky připraveným peptidem Buforinem P11L. Nejprve jsem prováděla počítačové simulace lipidových membrán a počítala jsem množství volné energie, které by bylo nezbytné pro vytvoření póru. Následně jsem prováděla experimenty.

Cílem mé práce bylo zjistit, jak různá lipidová složení membrán ovlivňují účinnost antimikrobiálního peptidu. Došla jsem k závěru, že účinnost námi studovaného antimikrobiálního peptidu je vyšší, když působí na membrány záporně nabité. Ale také jsem pozorovala rozdíly v chování na membránách se stejným nábojem, ale různým lipidovým složením. Neutrálně nabité membrány peptid nenarušoval.

Klíčová slova: antimikrobiální peptidy, interakce, modely buněčných membrán

Mechanismus aktivace buněk imunitního systému pomocí LPS sinic vodního květu

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Abstrakt: Kontaminace pitné vody sinicovým vodním květem a jeho výskyt na vodních plochách sloužících k rekreaci je významným problémem v České republice, ale i po celém světě. Po styku s kontaminovanou vodou se u lidí objevují různé závažné somatické potíže. Jedná se o vyrážky či střevní potíže. Zvýšená produkce prozánětlivých cytokinů může vyústit až v rozvoj chronických zánětlivých onemocnění. Tato práce studuje a objasňuje mechanismus, jakým endotoxiny lipopolysacharidy sinic a bakterií aktivují buňky imunitního systému, a to především makrofágy. Pro toto studium byly použity environmentální vzorky vodního květu z České republiky a metody molekulární biologie, tedy western blotting a ELISA. Získané výsledky naznačují, že lipopolysacharidy vodního květu aktivují v buňkách imunitního systému signální dráhy vedoucí k produkci prozánětlivých cytokinů (TNF-α a IL-6).

Klíčová slova: Vodní květ, sinice, LPS, cytokiny, Toll-like receptory, interleukin 6, TNF-α.

Sekce studentů bakalářských a magisterských studijních programů

Trimethylchitosan a jeho potenciál pro biomedicínské aplikace

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Velmi diskutovaným tématem poslední doby jsou nosiče léčiv a jejich využití pro cílenou distribuci aktivních látek. Světové firmy se snaží nalézt nejlepší kombinaci lékové formy pro požadovanou distribuci aktivních látek. Tato práce se zabývá konkrétním biopolymerem trimethylchitosanem (TMC), jež by v budoucnosti mohl najít své uplatnění v nosičových systémech na bázi inhalačního podání nebo jako hojící hydrogel.

Cílem předloženého příspěvku je studium interakcí trimethylchitosanu s opačně nabitými látkami s ohledem na jeho potenciální biomedicínské využití. Pro tyto účely jsou využity difúzní procesy v hydrogelových matricích prokazující interakci trimethylchitosanu s opačně nabitými sloučeninami. Byly navrženy jednoduché podmínky, jež co nejdůvěryhodněji simulují přirozené podmínky při prostupu léčiv. Porovnáváním transportních vlastností kladně/záporně nabitých barviv s kladně nabitým trimethylchitosanem v gelu dokážeme posoudit reaktivitu a bariérové vlastnosti tohoto unikátního materiálu. Další stěžejní metodou práce je reologie, jenž zaštiťuje pochopení mechanických vlastností připravených gelů a možnost stanovit jejich ideální metodu přípravy. Kombinací zvolených metod jsme schopni nastínit ideální podmínky pro přípravu gelů na bázi trimethylchitosan se záporně nabitou protilátkou.

EPR štúdium fotoindukovaných procesov zmesných fotokatalyzátorov *g*-C_3N_4:TiO_2

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Uvoľňovanie prchavých organických látok (Volatile Organic Compounds, VOCs) alebo oxidov dusíka (NOx) do ovzdušia predstavuje jeden z hlavných environmentálnych problémov súčasnosti. Fotokatalytická oxidácia znečisťujúcich látok, ktorá využíva fotokatalyzátory založené na polovodičových oxidoch kovov ako je TiO2, si získala pozornosť ako nízkonákladová metóda na ich elimináciu. Fotokalyzátory na báze TiO2 absorbujú žiarenie hlavne v UV oblasti a absorpcia viditeľného svetla je výrazne nižšia. V poslednom období sa testuje na odbúranie NOx z ovzdušia grafitický nitrid uhlíka g-C3N4, ktorý síce absorbuje žiarenie vo viditeľnej oblasti, ale energetická pozícia hrany jeho valenčného pása neumožňuje priamu tvorbu hydroxylových radikálov reakciou vody a fotogenerovanej diery. Na zlepšenie účinnosti sa ako vhodná alternatíva ukazuje príprava zmesných fotokatalyzátorov g-C3N4:TiO2, ktorých fotoindukované procesy sme preštudovali pomocou EPR spektroskopie. Dvojzložkové zmesné fotokatalyzátory sa pripravili sonifikáciou chemicky exfoliovaného g-C3N4 a komerčného P25 v rôznych hmotnostných pomeroch. EPR spektrá g-C3N4 v tuhej fáze merané pri laboratórnej teplote a 100 K potvrdili prítomnosť singletu s hodnotou g = 2,0033, ktorý je charakteristický pre grafitické nitridy uhlíka. Fotoexcitácia UVA a viditeľným žiarením spôsobuje nárast intenzity signálu, ktorý bol najvýraznejší pre g-C3N4 materiál upravený chemickou exfoliáciou, čo dokazuje, že tento proces zlepšuje jeho fotokatalytické vlastnosti. Schopnosť študovaných zmesných fotokatalyzátorov suspendovaných vo vode alebo dimetylsulfoxide generovať reaktívne paramagnetické častice počas expozície UVA a viditeľným žiarením sme sledovali EPR technikou spinových lapačov. Detegované spinové adukty sme identifikovali simulačnou analýzou, pričom typ aduktu a jeho relatívna koncentrácia závisela od zloženia reakčných systémov a od času expozície. Výsledky potvrdili, že zmesné fotokatalyzátory s vyšším obsahom oxidu titaničitého sú účinnejšie v systémoch, kde mechanizmus degradácie polutantov prebieha prednostne pôsobením hydroxylových radikálov a fotokatalyzátory s dominantným podielom g-C3N4 sú účinnejšie v systémoch, kde zohrávajú významnú úlohu superoxidové radikálové anióny (napr. rozklad NOx).

Biotechnologická produkcia a porovnanie vlastností poly(3-hydroxybutyrátu-co-4-hydroxybutyrátu) s poly(3-hydroxybutyrátom)

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Polyhydroxyalkanoáty (PHA) sú biologicky odbúrateľné polyestery plne syntetizované mikroorganizmami, ktoré majú veľmi širokú škálu chemických a fyzikálnych vlastností. Produkcia PHA v mikroorganizmoch je odozva na zvýšenie množstva uhlíkového substrátu, alebo na limitáciu esenciálnych živín v produkčnom médiu. Granule PHA sa ukladajú v cytoplazme ako prípadný zdroj živín na prežitie v stresových podmienkach.

Pojem polyhydroxyalkanoáty predstavuje množstvo rôznych polymérov, v tejto práci to bude konkrétne poly(3-hydroxybutyrát) (P3HB) a kopolymér poly(3-hydroxybutyrát-co-4-hydroxybutyrát) [P(3HB-co-4HB)]. P3HB je v súčasnej dobe dobre preskúmaný, jeho základné fyzikálne a chemické vlastnosti zahŕňajú teplotu topenia okolo 178°C, teplotu degradácie okolo 200°C a vysokú kryštalinitu (55-80%). Tieto vlastnosti nie sú ideálne pre priemyselnú výrobu pretože polymér je tuhý, krehký a teploty topenia a degradácie sú blízko pri sebe preto nie je tento polymér úplne vhodný na termické opracovanie. Na druhú stranu [P(3HB-co-4HB)] sa v týchto vlastnostiach výrazne odlišuje.

Pre produkciu [P(3HB-co-4HB)] boli vybrané 2 mikroorganizmy, prvým je kmeň Delftia acidovorans, pre ktorý je zatiaľ potrebné zoptimalizovať produkciu no podľa dostupnej literatúry má produkovať vysoké percentuálne zastúpenie jednotky P4HB a druhým je kmeň Cupriavidus malaysiensis, ktorý bol kultivovaný v Erlenmeyerových bankách a v bioreaktore s objemom 2 a 4 litre. Ako zdroj uhlíka bol použitý g-butyrolaktón a zdroj dusíka bol síran amónny. Pri kultivácií v bankách bola produkcia biomasy 0,052 g·l-1·h-1. Po 72 hodinách kultivácie v produkčnom médiu bola koncentrácia biomasy 3,7 g·l-1 z čoho zastúpenie kopolyméru v biomase bolo 72,8 hm.%. Vlastnosti kopolyméru sa ukázali ako vhodnejšie pre termické opracovanie, teplota topenia sa znížila na 154°C a kryštalinita sa znížila na 29,2 %. Vďaka týmto vlastnostiam sa stal kopolymér vhodný na spracovanie extrudáciou a boli z neho pripravené zatiaľ 2 filamenty pri teplote 160°C. Zastúpenie jednotky P3HB v kopolyméry bolo 88,6% a jednotky P4HB 11,4%.

Do budúcna je cieľom tejto práce pripraviť kopolymér s dostatočnou tepelnou

odolnosťou a vhodným zastúpením jednotiek P3HB a P4HB, ktorý bude možné použiť na extrudáciu a následne využiť pripravený filament do 3D tlačiarne.

Poďakovanie: Táto práca bola financovaná prostredníctvom projektu ORION. Program ORION získal finančné prostriedky z výskumného a inovačného programu Európskej únie Horizont 2020 na základe dohody o grante č. 741527.

Ďalej bola táto práca podporená projektom SoMoPro (projekt č. 6SA18032). Projekt získal finančné prostriedky z programu pre výskum a inovácie Horizont 2020 Európskej únie v rámci akcí Marie Sklodowska-Curie a je spolufinancovaný Jihomoravským krajom podľa grantovej dohody č. 665860.

EPR štúdium fotokatalytickej aktivity kompozitných fotokatalyzátorov TiO_2-Bi_2O_3

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Preštudovali sme fotoindukovanú tvorbu reaktívnych foriem kyslíka kompozitných fotokatalyzátorov s potenciálnou aktivitou vo viditeľnej oblasti, ktoré sa pripravili kombináciou TiO_2 nanotyčiniek s polovodivým β-Bi_2O_3 resp. $(BiO)_2CO_3$, ktorý zabezpečuje efektívnu separáciu fotogenerovaných nosičov náboja. Suspenzie fotokatalyzátorov pripravené vo vode alebo v dimetylsulfoxide sa študovali EPR technikou spinových lapačov počas in situ excitácie fotokatalytických systémov UVA resp. viditeľným žiarením. Při štúdiu fotokatalytickej aktivity sa použil spinový lapač DMPO (5,5-dimetyl-1-pyrolín N-oxid). Koncentrácia detegovaných spinových aduktov sa použila pri hodnotení ich fotoindukovanej aktivity. Zosyntetizované kompozitné nanomateriály vykazovali vyššiu aktivitu v oblasti UVA ako TiO_2 štandard P25. Vodné suspenzie pri koncentrácii 0,083 g/L vykazovali schopnosť zoxidovať samotný spinový lapač. Všetky kompozitné nanomateriály súčasne generovali radikály aj pri excitácii viditeľným žiarením. S cieľom zistiť optimálny pomer medzi oxidom titaničitým a oxidom bizmutitým, sme preskúmali tvorbu reaktívnych foriem kyslíka v suspenziách kompozitných fotokatalyzátorov s rôznym hmotnostným pomerom oxidov. Výsledky potvrdili, že v oblasti UVA a aj VIS sa najvyššie koncentrácie spinových aduktov pozorovali pre kompozity s vyšším obsahom oxidu bizmutitého, čo znamená, že vytvorenie kompozitu napomáha celkovej fotokatalytickej aktivite.

Kľúčové slová: kompozitné fotokatalyzátory; TiO_2; Bi_2O_3; EPR spektroskopia; technika spinov ých lapačov

Příprava a charakterizace mechanických vlastností artificiálních synoviálních kapalin

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Tato práce se zabývá problematikou optimalizace postupu přípravy artificiální synoviální kapaliny, který vychází z patentu US 8716204. Jako srovnávací matrice byla použita koňská synovie, která byla získána z kliniky chorob koní pod Veterinární a farmaceutickou univerzitou Brno (VFU). V rámci této práce byla provedena optimalizace přípravy synoviálních kapalin v několika dílčích krocích (způsob dispergace komponent, volba molekulové hmotnosti kyseliny hyaluronové, povaha a iontová síla použitého disperzního prostředí). Pro charakterizaci byla použita DLS mikroreologie, termogravimetrická analýza (TGA) a infračervená spektroskopie (FTIR). Postupem vycházejícím ze zmíněného patentu se povedlo připravit artificiální synovii, která vykazuje obdobné charakteristiky jako reálná synovie, což bylo potvrzeno jednak na základě provedené materiálové charakterizace i na základě vykonaných testů viskoelastických vlastností i stability.

Klíčová slova: synoviální kapalina, stabilita, mikroreologie, dynamický rozptyl světla, mechanické vlastnosti, komplexní viskozita

The Effect of the Side Chain Engineering on the Material Properties of Nature-Inspired N,N'-Alkylated Riboflavin Derivatives

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Group of naturally occurring materials, "flavines" (isoalloxazines), possesses a great versatility from a chemical point of view. These sustainable, biocompatible, non-toxic, and potentially low-cost materials play an important role as biological photoreceptors and redox coenzymes in the nature. Therefore, they have been already considered as bio-organic semiconductors for future bioelectronic applications. In this study, we are introducing nine different N,N'-alkylated flavine molecules which were synthesized by direct alkylation of already presented non-alkylated derivatives.

Alkylation was performed using corresponding alkyl halides or tosylates. After the purification via column chromatography or recrystallization, required new flavine derivatives were obtained in moderate yields. Afterwards, comprehensive chemical and physical characterizations were performed in order to evaluate the role of the modification of the initial alloxazine core by the π-conjugated system expansion and the effect of short linear, bulky, and oligoetheric substituents on the molecular properties.

Thin films of flavines were prepared using spin-coating and physical vapor deposition technique. The optical, electrical, electrochemical, and morphological measurements were done in order to determine material properties. Subsequently, we evaluate the potential applications of these unique molecules in organic electronic devices.

Acknowledgement: The work was supported by the Ministry of Industry project TRIO No. FV20022.

Keywords: flavines, π-conjugated molecules, nature-inspired materials, organic electronics, side chain engineering

Využití hroznových výlisků pro bakteriální produkci biopolymeru

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Vzrůstající zájem o ochranu životního prostředí a také obavy z budoucího vyčerpání ropy vedly vědce k bližšímu prozkoumání polyhydroxyalkanoátů. Tyto látky jsou jako jediné polyestery zcela biologicky syntetizovány. I přesto, že jsou biodegradabilní a biokompatibilní, mohou se díky svým mechanickým vlastnostem srovnávat s plasty produkovanými petrochemickým průmyslem. Jedním z typických představitelů těchto látek je poly(3-hydroxybutyrát-co-3-hydroxyvalerát), uváděný pod zkratkou P(3HB-co-3HV). Pro produkci tohoto kopolymeru byla zvolena bakterie Cupriavidus necator H16, jako uhlíkový zdroj byla použita čistá fruktóza. Po nastudování režimu přidávání kyseliny valerové na syntézu P(3HB-co-3HV), byla produkce daného kopolymeru provedena i v bioreaktoru. Vzhledem k tomu, že komercionalizaci těchto bioplastů brání především jejich vysoká cena, objevují se snahy tuto cenu snížit. K těmto účelům může sloužit vhodná volba uhlíkového zdroje. Substrát by měl být v ideálním případě obnovitelný a celosvětově dostupný. Hroznové výlisky – odpad vinařského průmyslu – jsou lignocelulózový materiál, ze kterého lze po enzymatické hydrolýze získat cukerný extrakt. Za využití tohoto alternativního uhlíkového zdroje a optimalizovaných podmínek syntézy P(3HB-co-3HV) bylo v Erlenmeyerových baňkách vyprodukováno 3,51 g/l tohoto kopolymeru a v bioreaktoru pak 5,06 g/l.

Poděkování: Táto práce byla podpořená projektem SoMoPro (projekt č. 6SA18032). Projekt získal finanční prostředky z programu pro výzkum a inovace Horizont 2020 Evropské unie v rámci akcí Marie Sklodowska-Curie a je spolufinancován Jihomoravským krajem dle grantové dohody č. 665860.

Poznámka: Tento materiál odráží pouze postoje autora a EU není zodpovědná za jakékoli použití rezentovaných informací.

Charakterizácia poranenia miechy potkana pomocou zobrazovania tenzora difúzie

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Poranenie miechy je častým dôvodom ochrnutia či straty citlivosti. Rozsah poškodenia resp. výsledný klinický stav určujú mnohé faktory, z ktorých najvýznamnejší je pravdepodobne miera integrity bielej hmoty. Zobrazovanie tenzora difúzie pomocou magnetickej rezonancie (DTI) je neinvazívna metóda, ktorá slúži na charakterizáciu tkaniva s vláknitou štruktúrou. Preto sme sa v tejto pilotnej štúdii pokúsili použiť metódu in vivo DTI na charakterizáciu tkaniva bielej hmoty v experimentálnom modeli kontúzneho poškodenia miechy potkana.

Techniku DTI sme použili v pilotnej štúdii kontúzneho poškodenia miechy na skupine dvoch potkanov. Poškodenie miechy sme kvantifikovali pomocou štyroch parametrov: frakčná anizotropia (FA), priemerná difúzivita (MD), axiálna difúzivita (AD) a radiálna difúzivita (RD) v segmente miechy s dĺžkou 2 cm. Výrazné zmeny v parametroch sme pozorovali v epicentre lézie a v menšej miere v jej okolí v porovnaní s kontrolnou vzorkou. 3D vizualizácia poškodených vlákien a stanovenie parametrov FA, MD, AD, RD boli realizované pomocou programu DSI Studio.

Metódu DTI sme použili na charakterizáciu a kvantifikovanie poškodenia miechy na skúšobnej vzorke zvierat. Neskôr bude metóda DTI použitá na väčšej skupine zvierat pri testovaní nových terapeutických postupov.

Metóda DTI je zdá sa perspektívna metóda, ktorá môže byť nápomocná pri identifikácii rozsahu poranenia miechy a pri vyhodnocovaní jeho priebehu v čase. Môže tak prispieť k úspešnej liečbe a pomôcť pri posúdení efektivity zvolenej terapie.

Využití modrého světla pro přípravu hybridních hydrogelových sítí s uplatněním v medicíně

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Cílem předložené práce byla příprava hydrogelu s hybridní chemicko-fyzikální sítí pomocí modrého světla z biodegradovatelného kopolymeru založeného na kyselině polymléčné a polyglykolové (PLGA) s polyethylenglykolem (PEG). Nový degradabilní hydrogel, připravený jak fyzikálním síťováním (při fyziologické teplotě 37 °C), tak i chemickým síťováním (pomocí modrého světla) by mohl být využit jako resorbovatelný kryt ran nebo jako injektovatelný nosič s postupným a velice dobře řízeným uvolňováním léčiv.

Termocitlivý triblokový PLGA–PEG–PLGA kopolymer syntetizovaný živou polymerací za otevření kruhu byl následně funkcionalizován anhydridem kyseliny itakonové za vzniku ITA/PLGA–PEG–PLGA/ITA makromonomeru citlivého jak na světlo, tak i na změnu teploty. Při teplotě 37 °C tvoří kopolymer díky hydrofobním interakcím micelární síť. Dvojné vazby kyseliny itakonové, která je navázaná na koncích kopolymerního řetězce, umožňují fotochemické kovalentní zesítění micel a zvýšení tak hydrolytické stability hydrogelu.

Syntetizované kopolymery byly charakterizované metodami GPC a ^{1}H NMR. Vznik fyzikální sítě při fyziologické teplotě byl potvrzen reometrem v místě křížení elastického a ztrátového modulu (G' a G''). Fyzikálně zesítěný ITA/PLGA–PEG–PLGA/ITA hydrogel byl následně, v přítomnosti hydrofilního netoxického fotoiniciátoru a pomocného síťovadla ozářen modrým světlem o vlnové délce 430–490 nm. Vzniklý hydrogel byl transparentní, ohebný, absorboval až 1376 % vody a ve fyziologickém roztoku při 37 °C byl stabilní 15 až 21 dní v závislosti na čase ozařování modrým světlem. Zesítěný hydrogel byl chemicky charakterizován pomocí ATR-FTIR, nicméně další analýzy jsou potřeba k podrobnějšímu pochopení principů nových typů hybridních hydrogelů z jednoho typu kopolymeru. Cílem je nastavení řízeného uvolňování bioaktivních látek z hybridního hydrogelu pomocí hustoty fyzikálně-chemické sítě.

Poděkování: Tato práce byla podpořena Ministerstvem školství, mládeže a tělovýchovy České republiky v rámci projektu CEITEC 2020 (LQ1601).

Klíčová slova: hydrogel, hybridní síť, fotopolymerace, termocitlivý kopolymer, modré světlo, hydrolytická stabilita

Včasné štádiá neurodegenerácie s anti-diabetickou terapiou skúmané na animálnom modeli lokalizovanou *in vivo* ^{1}H MRS

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Táto práca bola zameraná na meranie spektier mozgových metabolitov pomocou in vivo lokalizovanej protónovej magnetickej rezonančnej spektroskopie (1H MRS) a ich kvantifikáciu v dôležitom regióne mozgu, ktorý je zodpovedný za pamäť a učenie. Meranie a následná analýza spektrálnych dát bola realizovaná na animálnom modeli starnúceho mozgu s následnou anti-diabetickou terapiou. In vivo 1H MRS sme vykonávali na 4,7T magnete s využitím tzv. duálneho systému cievok (objemová cievka na excitáciu a povrchová na prijímanie signálu MR). Spektrá boli získané z oblasti ľavého hipokampu z elementárneho objemu (3x3x4 mm) pomocou sekvencie SPECIAL, ktorá zahŕňa aj potlačenie vody sekvenciou VAPOR. Táto metóda nám umožňuje pri danej intenzite magnetického poľa nameriať a kvantifikovať niekoľko dôležitých cerebrálnych metabolitov: celkový cholín, kreatín, kreatínfosfát, glutamát, glutamín, myo-inozitol (Myo-Ins), N – acetylaspartát (NAA) a taurín. V našej analýze sme vyhodnocovali len relatívne koncentrácie týchto metabolitov vzhľadom k celkovému kreatínu (Cr+PCr).

Prostredníctvom animálneho modelu metabolickej demencie - každodenným subkutánnym podávaním D-galaktózy do potkanov po dobu šiestich týždňov a kvantifikáciou 1H MRS dát sme sa snažili nájsť nielen vhodné biomarkery skorých štádií neurodegenerácie - sporadickej formy Alzheimerovej choroby (AD), ale zisťovali sme aj účinok terapie metformínom. Experimentálne zvieratá – (trojmesačné potkany kmeňa Wistar) boli rozdelené do 3 skupín. Prvá skupina s modelovanou metabolickou demenciou aplikovaná D-galaktózou (150mg/deň a neskôr bola dávka zvýšená na 220mg/deň). Druhej kontrolnej skupine bol aplikovaný metformín (200mg/deň). Tretia, tzv. liečená skupina s modelovanou metabolickou demenciou aplikovanáD-galaktózou a zároveň liečivom Metformín (200mg/deň). Aplikovaním D-galaktózy a následným liečením antidiapetickým liekom – Metformínom sme sa snažili poukázať na škodlivosť nadmerného používania cukru v potrave človeka a zároveň demonštrovať spojitosť demencie AD typu s diabetom typu 2.

Výsledky analýz pomocou dvoch kvantifikačných softvérov (jMRUI a LCModel) ukázali, že v D-galaktózovej skupine sa neuronálny marker NAA (ukazovateľ stredných a pokročilých štádií neurodegenerácie) nezmenil. Tento fakt nám signalizuje, že animálny model mal simulovanú neurodegeneráciu v skorých štádi-

ách, čo nám potvrdili aj in vitro biochemické analýzy a tiež behaviorálne testy. Korelujúce zmeny v oboch softvéroch sme zistili pri metabolite glutamát, práve jeho marginárne zvýšenie je spojené so zvýšenou úzkosťou v správaní sa zvierat, čo je tiež typické u ľudí v skorých štádiách demencie. Signifikantný nárast v jMRUI a marginárny nárast v LCModeli sme zaznamenali pri myo-inositole, ktorý pravdepodobne reflektuje tkanivový neurozápal, ktorý predchádza neurodegeneráciu a v literatúre sa považuje za marker skorých štádií AD. Jedinou nezhodou medzi softvérmi je marginárne zvýšenie cholínových rezonancií, ktoré sme zaznamenali len v LCModeli. Zmena tohto metabolitu je príznačná pre vaskulárnu formu demencie. V druhej skupine sme nezaznamenali žiadne signifikantné zmeny v koncentráciách metabolitov, takže toto liečivo nespôsobuje žiadne preukázateľné zmeny zdravým jedincom. V liečenej skupine sme takisto nezistili zmeny v koncentráciách cerebrálnych metabolitov. To znamená, že antidiapetikum metformín má priaznivé pleiotropné účinky na počiatočné štádia degenerácie mozgu a dokáže ho ochrániť pred negatívnym vplyvom D-galaktózy, pretože zvýšené hladiny metabolitov sa vrátili k norme.

Nakoľko všetky *in vivo* ^{1}H MRS merania a kvantifikácie metabolitov sa robili pred a po terapii na tom istom zvierati (mozgu), umožnilo nám to robiť párové testy, čím sa nám podarilo poukázať na spojitosť medzi sporadickou formou AD a diabetom 2. typu. Tieto naše výsledky by mohli mať priamy terapeutický potenciál v humánnej medicíne.

Reducing the Viscosity of Black Liquor by Modifying the Organic Fraction

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This work addresses the issue of reducing the viscosity of kraft black liquor. Black liquor is the spent aqueous solution from the kraft process in which pulpwood is transformed into paper pulp. It consists of organic material from wood and inorganic chemicals used in the process. In order to obtain these inorganic compounds for further processing, black liquor is submitted into numerous evaporation units until a required concentration of dry solids content is reached and it is then burned in the recovery furnace.

When black liquor is being concentrated, several problems are faced, including high liquor viscosities at high solids. To reduce the impact of high viscosity on heat transfer in the evaporator, methods such as heat treatment, oxidation of black liquor or addition of various inorganic chemicals have been developed.

This work proposes a new physical method of decreasing the viscosity of black liquor using high-frequency waves – ultrasound. The exposure of the black liquor to ultrasound would alter the bonding of the organic phase resulting in a change in viscosity. This hypothesis was tested through several experiments using samples of black liquor from one of Mondi's pulp mill from central Europe. We compared the black liquor from the concentrator before ash is dosed, called black liquor without ash, and black liquor with ash. The liquor with substantially lower amount of organic material, black liquor with ash, has a lower viscosity than the liquor without ash. Before the experiment, the samples were carefully heated up to a fixed temperature and then applied to the rheometer to evaluate the flow curves. Rheological properties such as shear stress and viscosity were measured with different shear rates for samples with and without the exposure to ultrasound. The duration of the exposure of ultrasound for first experiment was 5 minutes, and for the second experiment 10 minutes.

The viscosity of black liquor increases with dry solids content and decreases with the shear rate, meaning that black liquor acts as a pseudoplastic fluid. Further study and research are needed to fully understand the behaviour of the liquid.

Methodology for the optimization of LIBS analysis of soft tissues

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Biological tissues contain essential trace elements, which are known to have an important role in various metabolic processes taking place in the human body. In this work we focus on optimization of Laser-induced breakdown spectroscopy (LIBS) methods used for detection of these elements in soft tissues. Analysis of such samples using LIBS could be used for numerous biological applications in the future, such as utilization of listed trace metals as the potential biomarkers for cancer tissue diagnostics.

LIBS was applied to perform the elemental analysis of soft tissue samples – mouse kidneys. In order to get the optimum signal in the multi-element LIBS measurements of kidneys, the following experimental parameters: defocus, gas purge, atmosphere were adjusted, and signal to noise ratio response was studied. The process of optimization of experimental settings was described. Due to a different sample size and heterogeneity, a protocol of unification and mutual comparison was proposed.

Effect of carbon source on the microbial production of bacterial cellulose

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The worldwide production of wine in 2018 reached 292 million hectoliters. After the pressing of grapes for the wine production, grape pomace remains. Approximately 750 liters of wine and 260 kilograms of grape pomace is obtained from 1.3 tons of grapes. Grape pomace is a mixture of grape skins, seeds, and stems. The exact composition depends on the sort of grapes and the way of wine production. But pomace obtained from red or white wine production still contains a high concentration of sugar.

South Moravian region is known for its wine production so a relatively high mass of pomace could be available. Our research shows that the sugar extract from grape pomace could be used for the cultivation of Gluconacetobacter xylinus and the production of bacterial cellulose. This work shows an effect of pH, the type of cultivation (dynamic or static), and the kind of carbon source on the production of bacterial cellulose and its molecular weight.

Interestingly, the most effective carbon source was the grape pomace extract. The production of bacterial cellulose with 20 g/l of the sugar extract from the grape pomace was 13.5 g/l of bacterial cellulose. The reason is its composition (glucose, fructose, polyphenols, acids). The bacterial cellulose has unique properties compared to cellulose isolated from lignocellulosic materials such as high purity and mechanical strength. The use of bacterial cellulose is limited mainly to the medicine field because of its high price. However, also the applications in the food industry, textile industry, and electro-technique are known.

Our research is ongoing, and our nearest goal is to increase the production of the bacterial cellulose by using the fed-batch production and by optimizing the amount of dissolved oxygen in the medium.

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Zpracování Ramanových spekter pro *in vivo* diagnostiku karcinomu plic

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Karcinom plic je rozšířené a závažné onemocnění, jehož včasná a kvalitní diagnóza je jedním z klíčových faktorů určujících naději na přežití. V klinické praxi je zlatým standardem pro diagnózu karcinomu plic histopatologické vyšetření biopticky odebrané tkáně, které však klade vysoké nároky jak na zdravotní systém, tak na pacienta, pro kterého se jedná o invazivní zákrok. Vyšetření, které by umožnilo snížit počet biopsií s neprůkazným či negativním histologickým výsledkem má potenciál snížit zátěž pacienta, nemocnic i celého zdravotního systému. Slibným kandidátem na takové vyšetření se zdá být Ramanova spektroskopie, která je schopna zachytit patologické změny v biochemickém složení tkáně, k nimž dochází ještě před nástupem typických příznaků onemocnění, a tudíž je možné identifikovat raná, mnohdy ještě jednoduše léčitelná stádia karcinomu. Kombinace s vláknovou optikou potom otevírá možnost minimálně invazivního vyšetření se spolehlivým, vysoce specifickým výsledkem dosaženým v krátkém čase. Jednou z překážek pro klinickou aplikaci však v současnosti představuje nedostatečná automatizace zpracování spekter a absence jejich klasifikátoru.

V programovém prostředí MATLAB bylo proto vyvinuto algoritmické zpracování Ramanových spekter založené na filtraci s konečnou impulzní odezvou s odstraněním fázového posunu (Zero-phase FIR filtr). Tento postup umožnil při zachování srovnatelných výsledků automatizaci zpracování a tím redukci časové náročnosti o 94 % ve srovnání s běžně prováděným manuálním zpracováním dat. Metodami strojového učení byl dále vytvořen binární klasifikátor *in vivo* měřených Ramanových spekter plicní tkáně u pacientů s podezřením na karcinom plic, jehož správnost v současnosti dosahuje klinicky relevantní hodnoty 75 %. Práci koncovému uživateli pak zjednodušuje aplikace s grafickým uživatelským rozhraním, což do budoucna umožní vyhodnotit stav podezřelé tkáně přímo v průběhu bronchoskopického vyšetření.

Klíčová slova: Ramanova spektroskopie, *in vivo* diagnostika, zpracování spekter, automatizace

Organické polovodiče pre aplikácie v bioorganickej elektronike

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V súčasnosti patrí priemysel flexibilnej, tlačenej a organickej elektroniky medzi najvýznamnejšie a naj-dynamicky sa rozvíjajúce segmenty elektrotechnického priemyslu. S tempom vývoja úzko súvisí miera investícií v danej oblasti. V roku 2018 dosiahli ročné náklady technologických firiem do tejto priemyselnej sekcie hodnotu necelých 32 miliárd dolárov. Na základe štatistického odhadu IDTechEx sa táto suma v roku 2029 dostane na hodnotu 77 miliárd dolárov. Pri vývoji nových pokročilých materiálov pre organickú elektroniku je kladený dôraz najmä na zvyšovanie efektivity, zlepšovanie elektrických vlastností, znižovanie negatívneho vplyvu na životné prostredie, lacná výroba či miniaturizácia. Tieto požadované charakteristiky je možné dosiahnuť vďaka procesu modifikácie chemickej štruktúry a tým i vlastností organických materiálov na molekulárnej úrovni.

Bioorganická elektronika sa zaoberá vývojom a štúdiom organických elektronických zariadení, ktorých hlavnou funkciou je prevod biologických signálov na elektrické. Tento proces prebieha presne definovaným chemickým spôsobom, využíva sa preto na selektívne monitorovanie fyziologických procesov v bunkách, tkanivách či orgánoch. Pri takýchto funkčných zariadeniach je teda nutné použiť také materiály, ktoré dokážu viesť a zároveň aj spracovávať elektrónové i iónové signály. Tieto požadované charakteristiky spĺňajú napríklad vodivé polyméry, u ktorých zabezpečuje π-konjugovaný systém zvýšenú elektrónovú mobilitu. Zároveň majú aj unikátne optické, elektrochemické či mechanické vlastnosti. Ich veľký význam spočíva v jednoduchej, univerzálnej a nízko-nákladovej syntéze, pričom v priebehu tohto procesu je možná ich chemická funkcionalizácia pomocou modifikácií na molekulárnej úrovni, čím vznikajú funkčné deriváty s optimalizovanými vlastnosťami. Ďalšou výhodou vodivých polymérov je možnosť tvorby tenkých vodivých vrstiev s vysokou kapacitou náboja, rýchlym vedením nosičov náboja, nízkou impedanciou a dobrou adhéziou k substrátu. Z hľadiska aplikácií je dnes v organickej elektronike najčastejšie používaný polymér poly(3,4-etyléndioxytiofén) dopovaný poly(styrénsulfonát)-om, známy ako PEDOT:PSS.

Pri spojení so živými systémami ale dochádza k určitým obmedzeniam v aplikovateľnosti, ktoré spôsobuje najmä nízka biokompatibilita PSS. Pre rozšírenie aplikácií aj do oblasti bioorganickej elektroniky potom existujú dva možné prístupy. Prvý spočíva v nahradení PSS adekvátnym biokompatibilným dopantom. Ten druhý má základ v modifikácií PEDOT-ovej zložky syntézou funkčných derivátov EDOT monoméru. Táto alternatíva ponúka oveľa viac možností, keďže sa jedná o modifikáciu na molekulárnej úrovni, tak je možné pripraviť materiály na mieru pre konkrétne aplikácie.

Indirect 3D Printing of Bioceramic Scaffolds with Structured Macro Channels

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Porous materials are currently a subject of interest in modern tissue engineering. Scaffolds, made from ceramic materials, provide unique properties, such as biocompatibility, bioactivity, and biodegradability. A very important feature of the bioceramic bone scaffold is to support vascularisation, adhesion, and proliferation of bone cells. Nowadays, materials, that can release calcium and phosphate ions are bioactive and became very attractive in medical applications. The most used ceramic materials with these properties are hydroxyapatite, β-tricalcium phosphate, and whitlockite.

The ideal scaffold should have a pore size at least 200 μm for successful bone cell overgrowth (macro channels), but also smaller pore sizes are an advantage. The patient's bone is a three-dimensional virtual model that is easy to obtain using scanning techniques and then to print using additive technology. It is possible to prepare various constructions with defined channel geometry and shape. However, to achieve high porosity, mechanical stability, and defined macro channel geometry is still challenging.

Therefore, various 3D meshes were designed in the graphical editor with different arrangements of the macro channels. The 3D mesh was implemented to the form before freezing and casted by hydroxyapatite suspension. The mesh was removed by a sintering process and the macro channels were created by the presence of the 3D mesh. Various types of inner structured scaffolds with the same diameter in the green state were successfully prepared with diameter of macro channels in the range 540-600 μm.

It was experimentally found that the type of 3D mesh has an impact on the final mechanical stability of bone scaffolds. The mesh with helical structure has no significant effect on the mechanical stability of the resulting scaffold, it only influences the crack in the direction of the helix.

The porous scaffolds have a crucial problem in the bad mechanical properties, therefore they are used in low-loads places. Scaffolds with mechanical pressure of 0.2-0.7 MPa were prepared. The selected program did not achieve high porosity values than could be achieved with other rapid prototyping techniques.

The combination of these methods shows very good manageability with the controlled macro channels in the resulting highly porous structure (porosity over 70%). It is an extremely promising method for the preparation of bone scaffolds with different structures in the future.

Preparation and properties of poly(3-hydroxybutyrate) aerogels

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Poly(3-hydroxybutyrate) (P3HB) is a biodegradable semi-crystalline biopolyester synthesized and accumulated in bacterial cells in nutrient deficient conditions, except for carbon. Its biocompatibility renders P3HB also a promising material for tissue engineering, either in pure form or as constituent of a hybrid or composite material. However, besides biocompatibility, cell scaffolding materials need to meet a series of further prerequisites which include chemical, nanotopological, micromorphological and mechanical aspects. Interconnectivity, size and shape of voids for example are of immense importance for cell viability, ingrowth, signaling and propagation as well as diffusion of gases and metabolic products.

This presentation communicates the results of a study that investigated the preparation of free-standing shaped translucent gels from dilute solutions of P3HB and their onward conversion to P3HB cryogels and aerogels. Aiming to employ non-toxic and less volatile solvents, we tried to circumvent the use of common P3HB solvents like chloroform, dichloromethane or cyclohexanone and explored the solubilizing potential of DMSO in combination with a green cosolvents instead.

This approach turned out to afford nice colorless and translucent free-standing gels with solid contents of 2-2.5 % and porosities of up to 98%. The obtained products were converted to cryogels (after solvent exchange to water and fast freezing at -80°C) or aerogels (after solvent exchange to ethanol) using supercritical carbon dioxide (45°C, 9.5 MPa, 4h).

Preliminary nitrogen sorption experiments at 77K suggested a high interconnectivity of the voids and surprisingly high specific surface areas. These values will be verified till mid of November and will be supplemented by scanning electron microscopy and uniaxial compression testing of both cryogels and aerogels. *In vivo* degradation of the prepared P3HB scaffolds will the subject of future research.

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Sekce studentů doktorských studijních programů

Tématický okruh organická, enviromentální a biochemie

Toxicity of Metals in Urban Atmospheric Aerosol

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Atmospheric pollution is one of the most serious global problems. Atmospheric particulate matter (PM) is known as the source of several health effects. Metals constitute important class of pollutants that have received the attention of researchers all over the world. Metals are released into the atmosphere via both natural and anthropogenic (industrial activities, traffic) sources. Metals can enter the human body through inhalation causing several health issues (asthma, cardiovascular and respiratory diseases, lung cancer) due to the strong potential to be adsorbed on PM. Metal toxicity is closely related to their oxidative potential. The oxidative potential, defined as a measure of capacity of PM (or its compound such as metals) to oxidize target molecules, has been proposed as a metric that is related to biological responses to PM exposure. For determination of the particulate matter oxidative potential is currently used different assays.

The study of metals concentration in the atmosphere is important for understanding their environmental and health impacts. This study aimed to determine total metals concentration in PM_1 and $PM_{2,5}$ aerosol in winter, spring, summer, and autumn periods. The concentration of water-soluble fraction of metals was determined for a group of metals that was selected due to their ability to produce reactive oxygen species. After concentration measurement, some of the most important metals sources were calculated using Positive Matrix Factorization.

Keywords: aerosol, metals, PM_1, $PM_{2,5}$, source identification, oxidative potential

Effect of stressors on the PHB formation in the cyanobacterium *Synechocystis*

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Environmental pollution with plastics residues and threatening scarcity of fossil oil resources are among our most important challenges of the present. The production of the biodegradable polymer PHB (poly-3-hydroxybutyric acid) with phototrophically grown cyanobacteria may be a way to face these challenges by improving the sustainability of our society.

As cyanobacteria can fix CO_2 not only from the air but from exhaust gas, theoretically, such a biotechnological process can also contribute to a reduction of greenhouse gas emission. The concept sounds great, however, it is currently way too inefficient and uneconomical in bigger scale. Nevertheless, this approach can be very interesting for the future. For that reason it is necessary, to better understand the intracellular mechanisms of the PHB-synthesis in cyanobacteria; with the aim to achieve higher PHB yields.

Stanislav Obruca and his colleagues from the Chemical Faculty of TU Brno investigated the influence of some stressors on the PHB yields of the heterotrophic bacterium *Cupriavidus necator*. A higher PHB content in the cell helps them to survive stress conditions. In the Austrian-Czech joint project PHBecol we are searching for similar effects in cyanobacteria. For the experiments, we use two strains of the genus *Synechocystis*: PCC 6803 and CCALA 192.

Syn. PCC 6803 is a cyanobacteria model strain. It's genome is sequenced and there are an enormous amount of scientific publications about it. For *Syn*. CCALA 192 we can find only a handful of publications. But it is known from former projects (run at IFA-Tulln, Austria) that this strain has a better performance in cultivation and produces higher amounts of PHB than *Syn*. PCC 6803.

The project started in January 2019. Unfortunately there was some delay in our experiments, as we had to get rid of the bacteria contaminations which were delivered by the strain collections. In addition, the (non-axenic) cultures showed some non-reproducible growth behavior. Our basic research does not aim towards an increased PHB production only, we intend to study the behavior of the cultures by monitoring many parameters by physical and chemical methods. The presentation gives a short overview about the project, the challenge and about our approach to reach the project goals.

Keywords: cyanobacteria, PHB, *Synechocystis*, stress response

Urinary metabolites of organophosphorus flame retardants: A pilot study assessing exposure of Czech population

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Organophosphorus flame retardants (OPFRs) belong to the currently most widely used flame retardants in electronics, materials and consumers' products. Regarding their potential harmful effects on humans, e.g. potential carcinogenic and neurotoxic effects, their presence in the environment as well as in human body fluids is needed to be monitored. Unlike well-known brominated flame retardants (BFRs) which are persistent and are slowly excreted in an unmodified form, OPFRs undergo to rapid metabolism by hepatocytes to yield more polar derivatives: diesters, hydroxylated triesters or conjugates with glutathione and with glucuronic or sulfuric acid, which are easier excreted from the human body via urine.

The aims of this study were (i) to develop a simple, high-throughput method for the determination of six diesters of the most significant OPFRs, namely diphenyl phosphate (DPhP), bis(1,3-dichloro-2-propyl) phosphate (BDClPP), bis(2-butoxyethyl) phosphate (BBOEP), di-n-butyl phosphate (D*n*BP) and two isomers of dicresyl phosphate (DCPs) and (ii) to apply the new validated analytical approach within the pilot study on the analysis of their concentration in urine of the Czech population (n=142). Ultra-high performance liquid chromatography interfaced with tandem mass spectrometry (UHPLC-MS/MS) was utilized for the instrumental analysis of the target compounds.

The tested sample preparation procedures were extraction with acetonitrile and a simple "direct injection" approach. The recoveries were in the ranges of 80-115% with repeatability below 8% for both tested procedures. Although the latter procedure was easier, it was not used on the analysis of the real samples due to higher method quantification limits (MQLs) and more intensive clogging of the LC-MS/MS system. The MQLs for method based on extraction into acetonitrile ranged between 0.003-0.06 ng/ml urine. The newly developed and validated method was used for the analysis of urine samples within the pilot study in the Czech Republic. DPhP was the predominant OPFRs metabolite which was found in all samples with concentrations ranging between 0.10-2.89 ng/ml urine (median: 0.45 ng/ml urine). Compared to that, DnBP and DCP isomers were found on 16% and 9% of samples,

respectively and BDClPP and BBOEP were not found in any sample. Our results were lower compared to the studies from China (Zhang et al., 2018) or USA (Hoffmann et al., 2017) where the DPhP concentrations were up to 43 and 110 ng/ml urine, respectively.

Keywords: organophosphorus flame retardant metabolites, urine, LC-MS

Preparation and Characterization of Positively Charged Catanionic Vesicles

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This contribution is focused on the preparation and determination of the physicochemical properties of positively charged catanionic vesicles. Preparation of catanionic vesicles is based on mixing two oppositely charged surfactants, hexadecyltrimethylammonium bromide (HTMAB) and sodium dodecyl sulphate (SDS). After the counterions are removed from this mixture, the residue is called ion pair amphiphile (IPA) denoted as HTMA+DS– and is suitable to form a vesicular structuers when it is dispersed in aqueous environment. For preparation of positively charged catanionic vesicles a double chained dimethylammonium surfactants are often used. It can bring another benefit in enabling of interaction with negatively charged polymers (e. g. sodium salt of hyaluronic acid) and also it is usually added to improve system stability. For higher stability of these vesicles was added cholesterol. The presence of cholesterol is regard as the main factor to alter the physical properties. Due to the structure, these vesicles can serve like potential carrier for hydrophilic as well as hydrophobic substances.

Zeta potential and average size of positively charged catanionic vesicles was studied by dynamic light scattering (DLS) and electrophoretic light scattering. Average size of these vesicles was about 90 ± 10 nm and value of zeta potential was about 60 ± 10 mV. Solution of catanionic vesicles was stable only six days and during these days turbidity increased. Turbidity was checked by UV-VIS spectrophotometry. This work was supported by the Czech Science Foundation, project No. 19-14024J (GACR), and Ministry of Science and Technology, Taiwan, project No. MOST108-2923-E006-MY3.

Keywords: catanionic vesicles, ion pair amphiphile, dynamic light scattering, zeta potential

Influence of pH and Its Changes on the System of Phase-Separated Hydrogels

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The main focus of this work is to monitor how pH and its changes affect the properties of phase-separated hydrogels. Hydrogels were prepared by the interaction of polyelectrolyte and oppositely charged surfactant. In this work it was interaction of hyaluronan and Septonex. The studied pH range was 4-9. Changes in pH were simply observed and controlled by spectroscopic indicators. The main method for describing changes in the properties before and after pH change was rheology. The rheology was measured for all prepared hydrogels as well as for hydrogels that had changed pH. The pH values were always changed to the limit values of the selected range, i.e. four and nine. It has been shown that by changing the pH, the mechanical properties and partly also the internal structure of the hydrogel can be adjusted. The rheological results show that the hydrogels prepared at pH 9 and 7 seem to be the most interesting for their possible application use. Hydrogels prepared at pH 9 have the strongest bonds, but low permeability, and hydrogels prepared at pH 7, which in turn are very soft and are able to absorb large amounts of water. By changing the pH of the dispersion medium, it was possible to strengthen the formed bonds during the change to pH 9 and vice versa by changing to pH 4 the bonds were softened.

Keywords: hydrogel, pH, rheology, hyaluronan, Septonex

The Efficiency of Plant Compounds on the Viability of Probiotic Bacteria

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Probiotics, especially species as *Lactobacillus* and *Bifidobacterium*, are commonly used in dairy products and supplements to increase their amount in human gut and to help preserving homeostasis of gut microbiota. However, probiotics must survive transport through the gastrointestinal tract to large intestine with no harm and stay viable. Thanks to low pH and other factors probiotic viability might be decreased. Presence of plant compounds may positively affect probiotics and moreover using encapsulation techniques might protect both, plant compounds and probiotics, from environment negative effects [1][2][3].

The different types of sea algae and cyanobacteria were analysed for their dietary profile. Spectrophotometric methods were used to determine total and reducing sugar content, total phenolic and flavonoid content, antioxidant and antimicrobial activity in different types of extracts. HPLC/RI method was performed to specify percentage profile of sugars. Viability of probiotics and the effect of phenolic compounds on probiotic viability were determined by cultivation assay with strains *Lactobacillus acidophilus* CCM 4833 and *Bifidobacterium breve* CCM 7825T. Moreover, encapsulation techniques were performed.

Phenolic compounds from chosen plant extracts have shown positive effect on the growth of probiotics and, simultaneously, can inhibit the growth of pathogenic bacteria. Moreover, oil extracts are rich in total phenolic compounds, total flavonoids and have high antioxidant activity. Extracts were encapsulated into liposomes with high encapsulation efficiency. Prepared liposome particles with plant extracts were stable for more than 3 months.

Keywords: phenolics, probiotic bacteria, viability, antimicrobial activity, encapsulation

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Determination of Active Substances by HPLC-MS after Processing Waste from Wine Industry using Various Extraction Techniques

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In a world of science, it has been invested enormous effort in researching wine chemistry and its effects on human health. The winemaking process generates up to 20% of the total feedstock of waste in the form of grape pomace and grape cane. These intermediate products can comprise valuable bioactive substances such as resveratrol and viniferin which can be used in a whole range of sectors including medicine, pharmacy, cosmetic and food industry, thanks to their potential antioxidant activity.

To obtain the relevant amount of those bioactive compounds it is essential to use an effective extraction method. Due to that, a comparison of several different extraction techniques such as maceration, ultrasonic extraction, Soxhlet and pressured liquid extraction was performed. The yields of resveratrol and viniferin isolated from wine waste are crucially dependent on the conditions of used extraction technique. From this point of view, stability testing including light exposure, elevated temperature, and storage for longer time periods in the solution, represents the basis for optimizing conditions of extraction methods. For this purpose, a new HPLC-MS method was developed and validated. The method is proved to be accurate, reproducible and effective for the determination of resveratrol and viniferin content.

Depending on extraction time and used method, it was found that higher temperature is beneficial for better release of thermally more stable stilbenes such as trans-resveratrol and trans-viniferin but its application for prolonged time periods can be destructive. HPLC-MS results, confirmed by NMR, showed that, exposure to light leads to dimerization of resveratrol and photoisomerisation of trans form of viniferin, resulting in observable concentration increase of cis-viniferin form. According to this, the exposition to light during extraction setup will lead to extracts rich in cis-viniferin.

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A Comparison of Pretreatment Methods for Determination of Macroelements in Milk by ICP-OES

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Mineral elements have important roles in human body. They are involved in bone formation or membrane transport of essential substances, regulate different metabolic pathways and enzyme activities and support proper functioning of organ systems. Insufficient or increased intake of mineral elements above critical levels can cause various metabolic disorders that can result in damage to internal organs. Therefore it is necessary to ensure steady and regulated intake of mineral elements. Milk and milk products are a suitable source of mineral elements and other important nutrients in daily diet. Especially infants and adolescents require a higher intake of mineral elements for proper development of the skeletal and other organ systems. However, in the technological processing of raw milk the mineral content may decrease due to partial processes such as standardization of fat content or ultrafiltration, so it is necessary to monitor content of macroelements to maintain the desired nutritional value of final products.

Milk is a relatively complicated matrix because it is a polydisperse system of many components, including lactose, milk fat, proteins, enzymes, mineral salts and vitamins. It means that the sample pretreatment is a critical step to obtain precise results in elemental analysis. This study was focused on comparison of several commonly used methods, such as slurry dispersion, alkaline solubilization, wet ashing, dry ashing and microwave assisted ashing, for sample preparation before ICP-OES analysis. A reference material ERM® – BD150 with certified values of monitored macroelements was used as a model milk matrix for individual experiments. The slurry dispersion analysis is simple, fast and easy method for elemental analysis of milk matrix, but significant difference between measurements results and certified values of monitored macroelements except Mg was found. More corresponding results for K was obtained after acidification of slurry dispersion with nitric acid to final concentration of 1M HNO_3 and subsequent sonication, but in this case filtration was necessary before ICP-OES analysis due to precipitation of milk proteins. Moreover, lower concentration of P was measured after acid pretreatment of slurry dispersion. Another simple and reproducible pretreatment method is using TMAH reagent, which promotes the complete solubilization of the samples. On the other hand, TMAH presents problems of determination for some analytes, especially K. The most relevant results to certified values of macroelements were

achieved using wet ashing, dry ashing and microwave assisted ashing pretreatment methods. Then other factors should be considered, such as time, number of partial processes and cost, to choose the appropriate pretreatment method. However, the optimization of pretreatments for element analysis in complex matrix may still be a challenge.

Keywords: pretreatment methods, macroelements, ashing, milk, ICP-OES

Fluorescent Nanodiamonds Modified with Biocompatible Polymers

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In the past decade, sentinel node(s) mapping became standard procedure used in cancer diagnostics. However, agents commonly used in these applications, mostly blue dyes and radiotracers, still have several disadvantages. Fluorescence probes currently show the most promising results as potential alternatives. Fluorescent nanodiamond (FND) is a biocompatible material which exhibit unique optical properties. The origin of the nanodiamond fluorescence is based on artificially created nitrogen-vacancy (NV) centers. Emission maximum of NV centres is in near-infrared region (approximately 700 nm) which belongs to the tissue imaging window. NV centers are extremely resistant towards photobleaching. These properties make FND an ideal candidate for bioimaging applications. This work is focused on preparation FNDs coated with D-mannosylated polyglycerol for sentinel node(s) visualisation. Polyglycerol coating overcomes limited colloidal stability of FNDs in the biological environment and enables surface modification possibilities. D-mannose targets macrophages, which are abundantly present in the sentinel nodes. The functionalization with D-mannose was achieved using click chemistry (azide-alkyne cycloaddition). First, treatment with glycidyl propargyl ether provided alkyne-modified polyglycerol which was connected with azidated D-mannose via click reaction. The optimal polymerization and click reaction conditions was extensively studied. Resulting particles (both mannosylated and non-mannosylated) were highly stable in the high-salt condition (1M NaCl) and non-specific protein binding in FBS was completely eliminated. The mannosylated particles interacted specifically with macrophages and showed enhanced retention in mice lymphatic nodes, providing a clear imaging contrast.

Dependence of PEDOT:PSS Thickness on Transconductance of OECT

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The organic electrochemical transistor (OECT) plays an important role in modern bioelectronics. Its use in study of living cells physiology keeps this device very attractive and at the forefront of various bioelectronic devices. In a case of some bioelectronic applications, namely in sensing, the high gain of the OECT is needed. To evaluate the OECT gain the transfer characteristics are measured and the value of transconductance is calculated. It is known that the transconductance is strongly dependent on electrical resistivity and the thickness of the organic semiconductor film, as well as on the ratio of the width to channel length. To develop the OECT with high transconductance, an optimal thickness of the organic semiconductor and the length of the channel must be found. In this study, the effect of the electrical resistance driven by channel length and thickness of poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) film on the resulting transconductance of planar OECT was studied. It was found that the electrical resistance is decreasing with the increasing film thickness and simultaneously, the transconductance is increasing as expected. When the channel length is increased the transconductance decrease. Based on these findings, it was possible to develop the OECT with high transconductance and thus high sensitivity for e.g. living cells physiology studies.

Keywords: OECT, PEDOT:PSS, transconductance

Potato glycoalkaloids and their effect on soil ecosystem

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This paper focuses on potato glycoalkaloids and their impact on the soil environment and organisms that are commonly found in close proximity such as mice, Wistar albino rats, Syrian golden hamster, *Helix aspersa* snails, Colorado potato beetle and filamentous fungi (*Ascobolus crenulatus P. Karst*, *Alternaria brassicicola*, *Phoma medicaginis* var. *Pinodella* and *Rhizoctonia solan*). Several extensive studies of potato glycoalkaloids have been conducted over the last decades. From the very beginning - from determining the presence of solanine and chaconin in potato tubers, hulls and roots, researchers have shifted to monitoring their toxicity (as early as 1933), the limit dose, and especially the impact on human health. In recent years, they have been paying close attention as a potential therapeutic aid in the treatment of cancer, especially esophagus and stomach. The aim of this paper is to point out the need to study the fate of glycoalkaloids from an environmental point of view, namely how their presence and subsequent degradation affect the soil environment and organisms living in the soil environment and its surroundings as relatively little information is available, especially on their mechanism. degradation and decomposition intermediates. In the future, it is therefore essential to focus on how soil type of various physicochemical properties affects the degradation of potato glycoalkaloids - solanine, chaconin and the formation of their metabolites. So far, the effect of these pesticide-related toxins and their metabolites on commonly used compost worms such as the scented earthworm (Eisenia fetida), which are commonly found in soil and artificial composters, has not been reported. Planned studies for the future should contribute to a comprehensive understanding of the relationship between potato glycoalkaloids present in soil and the soil ecosystem.

Keywords: potato glycoalkaloids, solanine, chaconine, soil

Use of neonatal meconium for amphetamine-type drug screening in newborns

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Drug abuse during pregnancy has become an emerging public health problem with a large impact on the child's health. Drug-exposed newborns can even experience neonatal abstinence syndrome (NAS), a characteristic set of withdrawal symptoms which requires immediate medical attention. Drug screening in newborns forms an essential part of neonatal care, since only the timely detection of drugs can result in an effective NAS treatment. For this purpose, meconium (first fetal stool) has become the sample of choice. It is formed in fetus from approx. 12th gestational week and is then fully excreted after birth. As it contains a wide range of exogenous compounds accumulated during pregnancy, meconium can reveal fetal drug exposure from second and third trimester. However, it is a complex semi-solid matrix, and a proper sample pre-treatment is a critical step before the instrumental analysis.

The aim of this work was to develop and optimize a new meconium extraction technique based on principles of salting-out assisted liquid-liquid extraction (SALLE). The method optimization included selection of acetonitrile as an appropriate solvent and MS compatible ammonium salts as salting-out agents. We further developed and validated an LC-MS/MS method for detection of selected amphetamine-type drugs. Reversed-phase LC analysis was performed on an Agilent Eclipse Plus C18 column and MS method was carried out in a positive electrospray mode using multiple reaction monitoring (MRM) technique.

The presented SALLE method showed various advantages over the traditional extraction methods. We significantly reduced volumes of organic solvents with respect to conventional liquid-liquid extraction (LLE) and our method was less expensive and time-consuming than solid-phase extraction (SPE). Finally, the developed analytical method was tested on a set of real meconium samples, with positive findings of amphetamine, methamphetamine and methylone.

Keywords: amphetamines, meconium, SALLE

Evolutionary Engineering Approach for Enhancement of Growth Characteristics and Producing Capacity of Selected PHA Producing Microorganisms

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Polyhydroxyalkanoates (PHAs) are microbial polymers which could replace traditional petrochemical plastics due to their favorable properties such as biodegradability and biocompatibility. Moreover, properties of PHAs depend on monomer composition therefore materials for selected purpose could be produced. Application of approaches of evolutionary engineering could be used to obtain microorganisms producing PHAs with required properties. Method is effective for gaining microbial strains with suitable characteristics on phenotype level (e.g. more effective growth, better productivity, ability of utilization different sources of carbon etc.) with no requirement for knowledge of genetic characteristics. Selected microorganisms *Cupriavidus necator* H16 (CCM 3726) and *Halomonas halophila* (CCM 3662) have been exposed to several biotechnologically relevant stressors. *C. necator* H16 was exposed to presence of NaCl causing osmotic stress which represented environmental stress factor, to copper ions representing anthropogenic pollutant and to levulinic acid. Strain *H. halophila* was exposed to acetic and also to levulinic acid; components of hydrolysate of lignocellulosic biomass. Evolutionary experiments were provided using multiple serial transfers of cell cultures in Erlenmeyer flasks after 48 hours of cultivation. Except basic screening, selected preserved passages were characterized considering their potential of PHAs accumulation, effectivity of utilization of organic acids, testing of robustness and other differences between evolved strains and wild-type strains.

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Keywords: evolutionary engineering, polyhydroxyalkanoates, *Cupriavidus necator* H16, *Halomonas halophila*

Assessment of the drinking water treatment plant effectiveness via ecotoxicological tests and screening analyses

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The consequence of continuous environmental pollution is deteriorating of the quality of surface water. Raw water is being modified to drinking water by technological processes, and it is therefore necessary to put increased demands on the efficiency of these technological processes and their possible innovation. Drinking water treatment is still unable to treat the raw water perfectly, its pollution is only reduced to acceptable standards. For this reason, it is indispensable that the quality of drinking water is being checked regularly and at the same time the efficiency of individual technological processes of drinking water treatment is assessed. This includes screening analysis or eventually ecotoxicological tests.

Experimental part was focused on the evaluation of the efficiency of technological processes of drinking water treatment. Samples of raw water and samples of water after each treatment stage were collected at the drinking water treatment plant in the Czech Republic. These samples were subjected to ecotoxicological tests and screening analysis. Based on the ecotoxicological tests carried out on *Thamnocephalus platyurus*, *Lemna minor* and *Vibrio fischeri*, we can assume the emergence of harmful chlorinated by-products, which resulted to nearly 100% mortality of *T. platyurus*. Screening analyzes were performed after the extraction of specimens by the SPE method using HPLC/MS. The results of the screening analysis indicate, that the most effective method for the removal of hormonal substances is ozonization.

Keywords: Drinking water, sand filtration, ozone, GAU filtration, UV radiation, chlorination, hormones, ecotoxicology, HPLC/MS.

Assessment of the effectiveness of advanced oxidation processes via ecotoxicity tests

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Recently, an increasing problem in wastewater treatment is the insufficient removal of some organic pollutants. These substances can be toxic to the environmental components already in a small amount, either acutely or chronically. The goal is therefore to develop of such technologies that ensure their effective removal. One possibility is to use advanced oxidation processes. Advanced oxidation processes work on the principle of non-selective oxidation mediated by OH radicals. Several methods such as ozonation, O_3/H_2O_2 (Peroxone), UV/ H_2O_2 or Phenton´s reaction can by use to generate them. The aim of this work was toevaluate the effectiveness of the used advanced oxidation processes in wastewater treatment via ecotoxicity tests and assess if these processes couldn´t generate some new toxic substances.

Wastewater samples from WWTP Brno – Modřice treated by the ozonation and O_3/H_2O_2 on the pilot flow unit showed low values of acute toxicity for selected test organisms (*Daphnia magna, Thamnocephalus platyurus, Sinapis alba, Lemna minor*). The sample of wastewater was also treated by UV/H_2O_2 on laboratory circulation unit. In this case, there was an increase in acute toxicity on the testing organism *D. magna* and *L. minor* observed. The similar effect was observed in the test with the *D. magna* with the model water with selected pharmaceuticals treated by the same method. While the tests on the *L. minor* showed a reduction in toxicity.

Keywords: ecotoxicity tests, advanced oxidation processes, efficiency of treatment, wastewater

Simultaneous Determination of Trace Mercury, Cadmium and Lead in Fish Sauce Food Matrix by Diffusive Gradients in Thin Films Technique

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Fish sauces are popular seasoning liquid originating in south-eastern Asian cuisine, consisting of fermented fish, salt and additional ingredients. Fish used for production could be part of geobiochemical cycle of many contaminating metals, some of which could be potentially hazardous for human health if long-term consumed in larger quantities. Therefore, monitoring of fishery products is required for sustaining food safety and quality. Due to the relatively low concentration of metal contaminants, high saline content and complicated matrix effect, direct analysis of fish sauce by common analytical techniques could be challenging. Possible pre-treatment steps to avoid that, however, include considerable dilution of the sample. That could the concentration of analytes of interest to decrease close or below the limits of the instrumental technique used. In this work, the environmental passive sampling tool - Diffusive Gradients in Thin Films (DGT) technique utilizing Chelex-100 and Purolite S924 resin gel and is used for determination of dissolved mercury (Hg), cadmium (Cd) and lead (Pb) in fish sauce. The method was validated by two basic tests: a linear metal accumulation over time and the reciprocal diffusion gel thickness. Due to fish sauces' high salinity levels, the effect of the NaCl concentration on the determination of selected metals was also studied. Metal concentration in deployment solution and the mass of metal accumulated on resin gels and was analysed after elution by SF-ICP-MS. After that validation step, the DGT technique was used for the analysis of real fish sauce samples purchased in the retail network, where the content of hazardous metals did not exceed the limit set by the EU legislation for fishery products. Due to the preconcentration ability of DGT, much lower concentration levels of Hg, Cd and Pb could be detected, compared

to microwave digestion of sample combined with SF-ICP-MS analysis. Therefore, DGT offers a non-destructive alternative method for trace element analysis in complex food matrices.

Keywords: fish, food safety, DGT, cadmium, lead, mercury, fish sauce

The Role of Mango Peel Extract in the Synthesis of Silver Nanoparticles and Their Use in Food Packaging

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Nanotechnology is dealing with nanoparticle structures ranging from approximately 1 to 100 nm. These nanoparticle structures have unique optical, electronic, medicinal and magnetic properties. Metallic nanoparticles can be synthesized with the use of physical and chemical processes, but also environmentally friendly methods (green chemistry) can be used. Green chemistry is a simple, fast and eco-friendly alternative to well-known chemical and physical procedures.

Silver nanoparticles are non-toxic to humans and most effective against bacteria, viruses and other eukaryotic microorganisms at low concentrations. Leaf and fruit extracts of various plants have already been reported to have impressive ability to reduce silver ions into silver metallic nanoparticles.

The aim of this study was to synthesize silver nanoparticles using mango peel water extract and $AgNO_3$ solution, then to observe prepared silver nanoparticles visually and to characterize them by UV-VIS spectroscopy, dynamic light scattering (DLS) and scanning electron microscopy – energy dispersive spectroscopy (SEM-EDS). Finally, with the use of sonochemistry, the prepared silver nanoparticles will be applied in food packaging, and thanks to their very good antimicrobial properties the prolonged shelf-life of food products will be expected.

Keywords: silver nanoparticles, food packaging, antibacterial properties

The influence of addition of spent coffee grounds and their refining products on physical and chemical properties of a soil and a growth of *Lactuca sativa*

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Annual worldwide production of spent coffee grounds (SCG) is more than 8,5 mil tonnes. Most of this amount is landfilled or incinerated. However, after the different refinery processes (acid hydrolysis, extraction, defatting etc.) SCG could be used as a substrate for production of biodiesel, bioethanol or polyhydroxyalkanoates. Thanks to its elemental composition it also could be a potential soil enrichment material. The aim of this pilot study was to evaluate the influence of the addition of untreated SCG as well as its acid hydrolysed, defatted and oxidized forms to a base clay soil, which is due to its low content of phosphorus and potassium impropriate for plant cultivation. Samples of SCG were added to the base soil in 2% w/w. The influence of the addition of SCG samples on pH, conductivity and content of extractable elements (Ca, K, Mg, P, Al, Fe, Mn, Na, Cu, Cr) were determined. Cultivation of *Lactuca sativa* was carried out in all mixture of a base soil and SCG samples for 3 weeks. As a reference for measuring data, samples of base soil and base soil with addition of a commercial NPK fertilizer were used.

Measurements revealed significant effects on physical and chemical properties of soil. Decrease of pH and an increase in conductivity was observed in all tested mixtures. The lowest pH (6,57) and the highest conductivity (1295 $\mu S \cdot cm^{-1}$) were observed in acid hydrolysed SCG samples. In all soil samples, the significant increase up to 50 % of extractable Ca, Mg and Mn was observed. On the other hand, during 3 weeks the addition of SCG samples did not significantly enrich the soil by P and K. In the growth experiments it was found, that addition of the substrates did not significantly promote growth in comparison with control sample. Germination of seeds were completely inhibited in soils enriched by hydrolysed SCG. In defatted and oxidized samples, the early germination and the highest number of plants were observed. The deficiencies of P and K had a great impact on growth rate and visual appearance of cultivated *Lactuca sativa*. In comparison with the base soil with NPK addition, plants had pink colour and lower growth.

Due to the acidity of SCG, its application is more suitable to the alkaline soils. It can enrich the soil by Ca, Mg or Mn, but it is not able to supply P and K in relative short time. Its potential as a source of biogenic elements could be better utilized after composting or in a form of a bio-char.

Keywords: Spent coffee grounds, refinery, agriculture, soil, fertilizers.

Preparation and Characterization of Liposomal Complex for Inhalation Drug Delivery

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Nowadays inhalation is becoming a more and more popular type of drug administration thanks to avoiding degradation of protein–based drugs and the first–pass effect. In the frame of this contribution, we focused on preparation of a new type of inhalation drug delivery due to the combination of trimethylchitosan (TMC) and stealth liposomes. TMC allows the system pass after inhalation into the bloodstream by reversible opening of tight junctions in alveoli. Stealth liposomes could continue into the bloodstream where they have enough time for drugs releasing even for targeting.

The best liposome composition suitable for interaction with TMC is appeared to be phosphatidylcholine, phosphatidic acid, PEGylated phosphatidylethanolamine, and cholesterol. The electrostatic interaction between TMC and stealth liposomes was tested by dynamic light scattering and electrophoretic light scattering. After the addition of TMC to stealth liposomes solution, the average size of particles and value of zeta potential increased. These experiments proved the electrostatic interaction between TMC and phosphatidic acid despite the content of polyethylene glycol.

Keywords: inhalation, trimethylchitosan, stealth liposome, dynamic light scattering, electrophoretic light scattering.

Psychoactive Pharmaceuticals in the Environment

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The concern of the presence of pharmaceuticals in the environment is still a current topic of many studies. Pharmaceuticals in the wastewater are not completely removed in today's conventional wastewater treatment plants. Psychoactive pharmaceuticals represent a group of medicaments that presence in aquatic ecosystems could bring about some serious environmental and health consequences. Increased consumption of antidepressants, anxiolytics and hypnotics leads to higher environmental exposure and risks.

The connection between the presence of a certain group of psychoactive pharmaceuticals (antidepressants and anxiolytics) in the aquatic environment and some serious environmental problems have already been proven. Behavioural and physiological changes have been observed all around the world on various organisms.

The research focuses on Advanced Oxidation Processes (AOPs) as a removal method with emphasis on prescribed psychoactive pharmaceuticals in the Czech Republic (representatives of anxiolytics and antidepressants). Experiments show that AOPs could be considered as a reasonable method to remove target substances from water and wastewater. The effect of higher concentrations of these chemicals on activated sludge from a wastewater treatment plant was also investigated.

Acknowledgements: This work was supported by the specific research project No. FCH-S-18-5331 from the Ministry of Education, Youth and Sports of the Czech Republic.

Keywords: Advanced Oxidation Processes, Psychoactive pharmaceuticals, Water technologies

Sekce studentů doktorských studijních programů

Tématický okruh anorganická chemie, materiálové vědy a inženýrství

Porosity of a-CSiO:H films

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Thin films of tetravinylsilane or its mixture with oxygen gas were prepared by plasma-enhanced chemical vapour deposition (PECVD) operating in pulsed mode. The oxygen-to-total-flow rate ratio (0 – 0.92) and effective power (2 – 150 W) were the only variable deposition parameters. The films deposited on silicon wafer were analyzed by infrared spectroscopy to evaluate the chemical structure of the deposited material. Infrared transmission measurements were made using a VERTEX 80 vacuum Fourier transform infrared (FTIR) spectrometer (Bruker Optics, USA) in the wavenumber range of 400 – 4000 cm^{-1}.

The assignment of IR absorption bands was carried. According to this assignment, the intensity and the area of the absorption band corresponding to CO_2 vibrations increased with enhancement in oxygen flow rate and effective power up to 3 sccm and 30 W, respectively and then decreases with further increase in oxygen flow rate and effective power. Infrared spectra indicated the incorporation of CO_2 gas into the thin films, which could be due to porous structure of as-prepared thin films. To confirm this assumption, GISAXS analysis (grazing-incidence small-angle scattering) was performed. According to GISAXS analysis, the pore size is 4.1 nm.

Keywords: thin film, PECVD, FTIR,porosity

Preparation and Characterisation of Thin Films of Antimony Tin Oxide

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Liquid composition for antimony doped tin oxide sol-gel deposition was prepared. Inorganic precursors of tin and antimony and ATO nanoparticles were used (tin(IV) chloride, antimony(III) chloride). ATO nanoparticles were dispersed in composition. This composition was used for spin-coating deposition of thin films. Composition was shaken for 0 – 8 days on laboratory shaker with 1 mm glass marbles. Set of samples made of 1 – 4 layers was deposited from every shaking period composition. Sheet resistance of prepared samples were examined by four probe sensing. Lowest sheet resistance of 2,83 kΩ/sq was reached. RMS roughness and thickness was measured by contact profilometry and calculated. Roughness range was calculated to 1,0 – 1,4 μm for nonshaken composition set of samples and 0,2 – 0,4 μm for shaken composition sets o samples. Thickness of samples reached 1,1 – 3,6 μm depends on number of layers deposited. Samples were measured on X-ray diffraction (XRD). Transmittance and haze were measured and calculated by UV-VIS spectrometry with integration sphere. Transmittance was ranged between 65 – 82 % depends on wavelength with maximum at 550 nm. Haze of samples was in range of 1 – 6 % depends on wavelength of light measured with minimum at red area and maximum at blue area of Visible spectrum.

Keywords: antimony tin oxide, thin layers, spin-coating,

Microstructural Characterization of Plasma-sprayed 8-YSZ/NiCrAlY Duplex Coating on AZ31 Alloy

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This paper deals with the microstructural characterization of atmospheric plasma-sprayed (APS) 8-YSZ/NiCrAlY duplex coating sprayed on wrought AZ31 magnesium alloy. The surface morphology of AZ31 magnesium alloy, NiCrAlY bond coat and yttria-stabilized zirconia (8-YSZ) ceramic top coat was evaluated using the scanning electron microscopy. The microstructure of AZ31 magnesium alloy from the cross-cut was evaluated using the scanning electron microscopy an energy-dispersive spectrometer and using the light microscope (LM). The phase composition of 8-YSZ/NiCrAlY duplex coating layers was evaluated using X-ray diffraction analysis. The analysis showed that deposited NiCrAlY bond coat is formed by Cr,Al-rich γ-Ni solid solution and β-NiAl phase. The phases Ni_5Y and α-Al_2O_3 were observed in the bond coat's microstructure too. The ceramic top coat was predominantly formed by non-transformable tetragonal t'-ZrO_2. The microstructure of AZ31 magnesium alloy was changed after corundum-blasting and after the deposition of NiCrAlY bond coat and 8-YSZ ceramic top coat when compared to plain AZ31 alloy. These microstructural changes led to the changes in the microhardness values. The microhardness of NiCrAlY bond coat was determined on 563 ± 74 HV 0.01 and the microhardness of 8-YSZ ceramic top coat was 1246 ± 56 HV 0.01. The plain AZ31 magnesium alloy achieved the microhardness of 69 ± 2 HV 0.01.

Keywords: YSZ, NiCrAlY, yttria-stabilized zirconia, plasma spraying, AZ31, magnesium alloy.

Comprehensive Study of Novel Adamantane Asymmetrically-Substituted Diketopyrrolopyrrole Derivatives

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A series of three derivatives of 2,5-dihydropyrrolo[4,3-*c*]pyrrole-1,4-dione (DPP) was prepared by nucleophilic substitution of 1-(2-bromoethyl)adamantane chains. A typical limitation of this type of reaction is its very poor selectivity, leading to the formation of *N*,*O*'- and *O*,*O*'-alkylated byproducts. Adamantyl side chain is a significant member of bulky alkylating agents first used for this purpose by our group 2 years ago. The main aim of this work was to synthesize and isolate all three possible products and to provide a comprehensive study of their properties and applications in perspective areas of organic electronics.

The significant influence of adamantyl side chains on the final properties of the *N*,*N*'-alkylated derivative has already been described by our group. Adamantane chains induce π-π interactions between the conjugated DPP cores through adamantyl-adamantyl stacking, which causes extraordinary interesting arrangement of the molecules leading to exceptional ambipolar characteristics.

In this work it was discovered that adamantyl chains has also a significant role in the crystallinity of *O*-alkylated derivative. Furthermore, optical properties were investigated for all prepared derivatives, both in solution and in thin layers. The position of alkyl chains in the DPP molecule significantly affected both absorption and fluorescence emission spectra. The thermal stability of *N*- and *O*-alkylated derivatives also differed significantly. DSC measurements revealed that the *O*-substitution caused a decrease in the thermal stability of DPP derivatives compared to *N*-alkylated. On the contrary, adamantyl side chain as a rigid alicyclic substituent contributed very effectively to the increase of melting point and thermal stability compared to other known alkylated DPPs by linear or branched alkyl chains. The results of this work surely provide novel insights in the development of DPP-alkylated regioisomers and their thermal and optical properties.

Keywords: diketopyrrolopyrrole, alkylation, adamantane, regioisomers, asymmetrical

The Effect of Polymer Microfibers on Rheological and Mechanical Properties of Calcium Phosphate Bone Cements

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The proposed master's thesis focuses on mechanical and rheological properties of biodegradable polymer-calcium phosphate bone cement composite reinforced with PCL (poly(ε-caprolactone)) and PCL-Pluronic polymer microfibers.

The theoretical part describes bone structure, the evolution of bone cements and structural additives. In the experimental part, synthesis and characterization of PLGA-PEG-PLGA thermosensitive copolymer and α-tricalcium phosphate powder is depicted as well as microfibers preparation technique. Copolymer aqueous solution was used to counteract the paste limited injectability. Liquid to powder (L/P) ratio of 0.5 ml/g was used for all of the samples. The two different mixing techniques were used in cement preparation to modulate the sample's porosity. PCL and PCL-Pluronic fibers used to reinforce the cement were added in the amount of 1, 3 and 5 wt. % to the total mass of cement paste. Prepared pastes were studied at the laboratory (23 °C) and under physiological conditions (37 °C) using dynamical rheological analysis, to establish the workability and setting of the paste. Samples for the rest of the analyses were enabled to set at physiological conditions for 10 days. Afterward, mechanical parameters like compressive strength, elastic modulus and diametric tensile strength of dried and in some cases hydrated samples were tested. Porosity was established using micro-computed tomography. Scanning electron microscopy was used to study microstructure and fiber incorporation into a ceramic matrix. Presence of fibers was semi-quantitatively studied using Fourier transformed infrared spectroscopy. X-ray diffraction provided data about powder phase transformation and mineralogical aspects of cement. Individual sample performances were evaluated and compared.

As a result, addition of either hydrophobic PCL or amphiphilic PCL-Pluronic fibers into polymer-phosphate cement slightly increased compressive strength where PCL-Pluronic modified fibers performed better. Therefore was concluded, that polymer-phosphate bone cement reinforced with microfibers is promising candidate for surgical practice.

Keywords: calcium phosphate bone cement, α-TCP, PLGA-PEG-PLGA thermosensitive copolymer, biodegradability, fiber reinforcement, mechanical properties, rheology

Spectroscopic changes in gelatin photographs after plasma treatment

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Gelatin photographs, as an important part of cultural heritage, are the most prevalent in photographic collections. New non-destructive treatment options were invented in the protection of cultural heritage. Some information regarding to use of low temperature atmospheric plasma in the field of cultural heritage objects, including photography, has been published over the last few years. The use of plasma seems to be a perspective method for both - photographs decontamination and optical properties improvement. At this point it is necessary to identify the effect on long term gelatin photographs stability.

The aim of the work was to investigate degradation effect of the low–temperature ADRE plasma (Atmospheric Discharge with Runaway Electrons) in nitrogen atmosphere on barytic photographic paper FOMABROM N 112 (normal) from Forma Bohemia (Hradec Králové). We made three series of photographic samples with different optical densities (D_0=0.075, D_0=0.272 and D_0=2.02). Plasma settings have been used (E = 0,3 J; f = 2000 Hz; gas flow = 6 l/s) with the aim to achieve optimal parameters of the plasma treatment, where no material damage occur.

We had achieved the characterization of the prepared samples, their alteration as a result of plasma processing, as well as their alteration during accelerated weathering in Q-Sun chamber. These processes were recorded by ATR FTIR spectroscopy and densitometry. During all plasma settings in the ATR FTIR spectrums, we observed the decrease in absorption band of Amide I (1635 cm^{-1}), Amide II (1537 cm^{-1}) and increase in the absorption band of Amide III (1337 cm^{-1}), while these results were recorded already during the short periods of plasma processing. We found out, that plasma surface treatment also had an impact on the increase of the ratio of bands AI/AII, which is one of the most important indicators of the hydrolysis of collagen materials. However, we observed that measurement of ATR FTIR spectrums of plasma treated samples, repeated tests after one day and after seven days showed a decrease in the ratio of AI/AII. This would mean that the plasma effects have a physical nature. In addition, we found out also that plasma surface treatment of the sample does not have any impact on its light stability.

Keywords: black-and-white silver gelatin prints; ADRE plasma; accelerated aging; ATR FTIR

Silicon Carbide Shell and Tube Heat Exchangers for Scrubbering Processes for Cooling

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The processes of cooling by shell and tube heat exchangers for subsequent application in processes of removal of gaseous air contaminants via liquid absorber is the major topic of the presented work. The aim of the work was to verify both the theoretical computational relations and the theoretical convenience of silicon carbide as a heat transfer surface material compared with traditional borosilicate glass material.

Heat transfer on semi-operating shell and tube heat exchangers with baffles and glass or silicon carbide heat exchange surface was examined by cooling the humid air by 50% propylene glycol in tubes having an inlet temperature ranging from 0 to 6 °C. For the five laminar coolant flows and the three air flows in the transition area, input and output flow temperatures including relative air humidity were measured.

Due to the low local air heat transfer coefficient caused by low ventilator power, differrences in exchanged heat between the exchangers were negligible, although silicon carbide has two orders of magnitude better thermal conductivity than glass. Nevertheless, much higher efficiency was performed by the carbide heat exchanger because the difference between air outlet temperature and liquid inlet temperature was one and a half times higher for the glass heat exchanger. That was reflected in a decrease in mean temperature difference, which resulted in a 16 % higher experimental heat transfer coefficient compared with the glass surface.

The theoretical model using the *j* factor, the correction factors for the baffles, and the correction for air humidity condensation have proven to be appropriate. For the glass surface, for the highest air flow rates the model gives an appropriate heat transfer coefficient; at lower flow rates it gives slightly higher values. For the silicon carbide surface, it gives a lower heat transfer coefficient because the model failed to consider a lower mean temperature difference. The results also evaluate the heat loss through the shell and the heat exchanged in addition by air humidity condensation.

The following direction of work will be the experiments with coolant temperature below 0 °C. Indeed, achieving low temperatures is crucial to increasing the efficiency of the separation of gaseous impurities from gas into liquid using a scrubber. The basis of this idea is the temperature dependence of the Henry's law constants.

Keywords: shell and tube heat exchanger, heat transfer, cooling, humidity condensation

Study of Chemical Processesin Extraterrestrial Atmospheres

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The presented work deals with laboratory simulation of chemical processes reflecting atmospheric composition of exoplanets under conditions that are close to the real conditions. The chemical processes initiated by electrical discharges in prebiotic atmospheres became a hot topic during the last decade because of extensive discovering of exo-planets. The biggest atmospheric data collection is about Saturn's moon Titan atmosphere is composed mainly from nitrogen and methane at low temperature of about 94 K and pressure about 1.5 atmospheres at its surface. The presented contribution gives the first measurement of the main composed formed in glow discharge at atmospheric pressure in nitrogen-methane gaseous mixture containing traces of oxygen and carbon dioxide at the relevant temperature. Results show very complex chemistry in these mixtures leading to the formation of currently considered direct life precursors like formamide.

Keywords: Extra-terrestrial planets, Titan moon, proton transfer time of flight mass spectrometry

Effect of adamantane substitutions on para-bis(2-thienyl)phenylene solid-state organic luminescent dyes

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IDTechEx Research finds that the total market for printed, flexible and organic electronics will grow from $41.2 Billion in 2020 to $74 billion in 2030. The majority of that is OLEDs, printed biosensors, printed conductive layers. On the other hand, stretchable electronics, logic and memory, flexible batteries, organic solid-state lasers, materials for medical treatment and diagnosis, optical fibers, solid state dye-labelling for DNA and capacitive sensors are much smaller segments but with strong growth potential. The development of new materials for abovementioned applications attracts interest due to the wide range of their applications. Para--bis(2-thienyl)phenylene as a dye represent perspective alternative for application in abovementioned fields. Here, we focus on the effects of various substitutions on the phenyl and thiophenes units. Incorporation of electron-withdrawing fluorine atoms results in HOMO and LUMO energies tuning and in molecular organization. On the other hand, solubilizing groups on thiophene units have impact on solubility, thermal and chemical stability and self-assembly what has a crucial effect for the device's fabrication and industrial applications. For example, substitutions on the thiophene units with adamantylethyl groups significantly increased melting point from 55 °C to 250 °C and photoluminescence quantum yield up to 50 %.

With regards to the possibility of well-targeted chemical modifications for the individual purposes, these molecules are determined for the use in organic electronics.

Keywords: adamantane, organic electronics, photoluminescence quantum yield

Diketopyrrolopyrrole (DPP) Pigments as Candidates for Charge Transport Layers in Perovskite Solar Cells

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Interface engineering in perovskite solar cells (PSC) plays a crucial role in achieving higher efficiencies as well as stability. Recent publications show that insertion of organic material-based interlayers into the structure of inverted PSC can significantly improve their performance. Diketopyrrolopyrrole (DPP) based semiconductor pigments are interesting candidates for such applications. These materials have been widely studied in various optoelectronic devices and therefore it is expected that they can possess desired properties. Moreover, use of DPP based pigments can offer possible enhancement of stability due to their inherent hydrophobic nature, thus can form a shield against moisture invading perovskite material.

In this study, we choose four DPP-based molecules and thoroughly investigate their optical and electronic properties to assess the feasibility of these materials as charge transporting layers. We carried out cyclic voltammetry and field effect mobility measurements to investigate their electronic properties. Optical properties were also investigated by absorption and photoluminescence spectroscopy. To gain insight into morphology of vacuum evaporated thin films, atomic force microscopy images of their surface were obtained. Photoluminescence quenching experiments were conducted on samples combining perovskite and pigment layers to evaluate their interaction.

Keywords: pigment, diketopyrrolopyrrole, charge transport layer

Mg-based Materials Prepared by Powder Metalurgy Method

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Magnesium and Mg alloys are suitable materials for lightweight applications because of their high specific strength. Currently, the conventional preparation methods, such as gravity and die casting are used for the preparation of these materials. Powder metallurgy methods offer the possibility of improvement of mechanical properties and corrosion resistance due to the introduced plastic deformation during the preparation. The materials for microstructure and chemical composition evaluation were prepared from the Mg-Zn powder mixture (1, 2, 3 and 5 % wt. Zn). The hot pressing method at 400 °C under 500 MPa was used for compaction of metal powder mixtures. Microstructures of the prepared materials were analyzed in terms of scanning electron microscopy. The chemical composition of processed materials was analyzed by energy-dispersive X-ray spectroscopy and verify by X-ray diffraction. At the temperature of 400 °C the sintering is supported by the presence of a liquid phase. Consequently, the microstructure is formed by magnesium matrix and network of $Mg_{51}Zn_{20}$ phase.

Keywords: magnesium, zinc, powder metallurgy

Synthesis of Organic Perovskites for Photovoltaics Applications

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This contribution is focused on the study of the synthesis of halide perovskites as the first step in the preparation of solar cells. Individual crystals and layers were prepared by inverse temperature crystallization (ITC). Perovskite solutions were prepared from halide salts and a suitable solvent (DMF, GBA) in a heated oil bath. Methyl-ammonium-lead bromide and iodide, formamidium-lead bromide and iodide and phenyl-ethyl-ammonium-lead iodide perovskites were prepared and their XRD patterns and SEM images were obtained. Perovskite bromide has proven to be the best stability under normal laboratory conditions. Crystallization of perovskite bromide was easy and spontaneous after reaching eighty degrees Celsius, and individual crystals of two millimeters in size grew. The high quality of these crystals was demonstrated by XRD, where the diffraction patterns contained only strong diffraction maxima of the major crystallographic planes. Perovskite iodide crystals showed higher oxygen and moisture sensitivity than bromide ones. In the case of iodide perovskites, two different types of crystals were observed and XRD patterns showed poor quality in terms of crystallographic plane positions. The crystallization method by seeding was used for formamidium-lead iodide and for the combination of formamidium and methyl-ammonium iodide. These samples crystallized only in the form of very small crystals, so seeding was necessary. The novelty of our experiments was the preparation of phenyl-ethyl-ammonium-lead iodide by ITC method. Although individual crystals of acceptable size were not achieved, thin films were successfully prepared. In summary, the results presented in this work showed the possibilities of crystallization of perovskite halides and the conditions under which it is possible to prepare single crystals of a size suitable for further photoelectrochemical experiments. The crystallization ability of the Perovskites depended on their composition, some of the Perovskites needed seeding. The stability of crystals depended on atmosphere composition and temperature, bromide perovskites were more stable than iodide ones.

Keywords: halide perovskite, perovskite synthesis

Dependence of PEDOT:PSS Thickness on Transconductance of OECT

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The organic electrochemical transistor (OECT) plays an important role in modern bioelectronics. Its use in study of living cells physiology keeps this device very attractive and at the forefront of various bioelectronic devices. In a case of some bioelectronic applications, namely in sensing, the high gain of the OECT is needed. To evaluate the OECT gain the transfer characteristics are measured and the value of transconductance is calculated. It is known that the transconductance is strongly dependent on electrical resistivity and the thickness of the organic semiconductor film, as well as on the ratio of the width to channel length. To develop the OECT with high transconductance, an optimal thickness of the organic semiconductor and the length of the channel must be found. In this study, the effect of the electrical resistance driven by channel length and thickness of poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) film on the resulting transconductance of planar OECT was studied. It was found that the electrical resistance is decreasing with the increasing film thickness and simultaneously, the transconductance is increasing as expected. When the channel length is increased the transconductance decrease. Based on these findings, it was possible to develop the OECT with high transconductance and thus high sensitivity for e.g. living cells physiology studies.

Keywords: OECT, PEDOT:PSS, transconductance

The comparison of the effect of Zinc compounds on hydration of ordinary Portland cement

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The content of heavy metals in various secondary industrial products and alternative fuels increases with the ecological push for reuse of waste materials and recycling. This effect is especially visible in the Portland cement properties. The cement production often involves burning of old tired as fuel and source of iron oxide and ground communal waste or industrial waste sludge as cheap fuel. The burning of waste in rotary kiln introduces heavy metal into cement clinker that have adverse effects on the properties and use of cement. Zinc has been proven to drastically increase of induction period of cement setting. The negative effect of zinc compounds on hydration of ordinary Portland cement was measured by isoperibolic calorimetry. Zinc was added to the cement in the form of two soluble salts of Zn(NO3)2 hydrate, ZnCl2 and a poor soluble compound ZnO. The concentration of zinc added was chosen as 0.05, 0.1, 0.5 and 1 mass %. The results show significant retardation of cement hydration with increasing zinc content with ZnO causing most drastic increase in induction period.

Keywords: Portland cement, Hydration, Zinc, Heavy metals, isoperibolic calorimetry

Synthesis of Novel N,N'-Alkylated Riboflavin-Inspired Conjugated Bio-Organic Semiconductors

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Biologically inspired molecular engineering is a promising way towards green, cheap, bio-compatible, non-toxic and versatile materials for future bio-organic semiconductor science and technology. In addition, ability to tune molecular structure allows improving of the stability and performance of the original material. As an example, flavins are one of the most structurally and functionally versatile redox centers in nature that act as cofactors in a wide range of biological transformations and electron-transfer reactions.

Herein we demonstrate an extended series of the recently published biocompatible flavin derivatives incorporating various fused or non-fused aromatic moieties attached to the pyrazine core. Moreover, the proposed synthetic strategies offered the access to various symmetrically and unsymmetrically alkylated flavin derivatives with wide structural portfolio of introduced alkyl substituents. Careful tailoring of the structure by π-system expansion and N-alkylation provides controllable physicochemical properties such as progressive light absorption, high thermal stability, improved solubility and tunable molecular packing. Comprehensive studies of physic-chemical properties have been performed and moreover, bioassays showed promising biocompatibility and stability of the selected flavins allowing for their possible applications in organic bioelectronics.

Keywords: flavins, π-conjugated molecules, bio-inspired materials, organic electronics

Organosilica binders for nanoparticles

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Nowadays there is a problem with anchoring of photocatalytic layers, which would not have to be cured at high temperatures. Therefore, a support binder is added to the photocatalyst itself. This work deals with the preparation of polysiloxane binders to serve as a support for anchoring photocatalytically active layers containing titanium dioxide. The primary aim of this study is to compare the properties of several polysiloxanes, differing in composition and method of preparation. The work focuses on the synthesis of polysiloxane binders containing various organic residues such as methyl, propyl and phenyl. The characterization of elemental composition and polysiloxane agglomerates in solution will be performed. Subsequently, the incorporation of binders into TiO_2/polysiloxane compositions with the photocatalytically active layers will be prepared and the methods of a polysiloxane mineralization in such layers up to SiO_2 will be investigated. The mineralization will be performed by UV radiation, plasma and thermal treatment. FT-IR and thermal analysis will monitor the polysiloxane mineralization. Finally, the layers will be subjected to a photocatalytic efficiency test.

Keywords: organosilica binder, polysiloxane, TiO_2, TiO_2/SiO_2 hybrid composition material printing, UV, plasma

Brookite Nanoparticles identification in Biphasic Photoactive TiO_2 using MCAA as chelating solution

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TiO_2 as catalyst still presents some limitations regarding its photocatalytic activity. Three different crystal forms exist. Anatase, Rutile, and Brookite. However, reports from brookite phase are still scarce. The Anatase-Brookite Nanoparticles represent a great perspective in water quality technologies at visible light. Significant progress has been made in the research of TiO_2 nanoparticles based on the modification of their crystal structure and particle size. The presence of brookite helps to retarded recombination of holes and accumulation of electrons in the conductive band leading to increasing the oxidation of organic substances and benefits oxidation-reduction processes. So that, structuring a cooperative behavior between the anatase and brookite phases is an important characteristic of TiO_2 catalyst when is applied in "green" technologies. Common attempts how to synthesize brookite have been widely described in literature. One of them is the hydrothermal synthesis which is simple and cost-efficient and allows to improve crystallinity in comparison with other methods (high-energy synthesis methods such as sputtering and pulsed laser deposition-PLD). The use of chelating agent is considered an important factor that influences the crystallography of the biphasic system subsequently prompting the photocatalytic activity of the material and is assumed that under it is developed a simultaneous complexation and hydrolysis of the precursor, generating a slow polycondensation of Ti-OH or Ti-OH_2^+ bonds to form a TiO_6 octahedrons that share corners and edges, which could facilitate the formation of brookite nuclei. Complexe synthesis of TiO_2 biphasic (BP) nanoparticles was performed, by the use of Titanium Isopropoxide (TTIP) as a precursor and Monochloracetic acid (MCAA) as a chelating solution at low-temperature.

Different analytical methods were used for the characterization of crystallography, microstructure and chemical composition of the synthesized TiO_2 BP nanopowder. Such as X-ray diffraction (XRD), Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM) which reveals the presence of both phases (Anatase and Brookite) with the content of brookite between 10 – 30 % and crystal size about 6-14 nm. X-ray photoelectron spectroscopy provided the atomic concentrations of Ti 2p, O1s, C1s and the deconvoluted binding energies for Ti 2p. Other physicochemical properties like particle size distribution were determined by Dynamic Light Scattering (DLS) which revealed mean diameter of 247.5 nm. The surface area of the nanoparticles was measured about 200 m^2/gr by multipoint

Brunauer-Emmet-Teller (BET) method. The characterization reveals that the synthesis under presence of MCCA as chelating solution is possible to obtain TiO_2 Anatase-Brookite BP nanoparticles. Finally, the photoactivity of a TiO_2 BP system was proof by spectrophotometry performed with the decomposition of the organic pollutant AO7-Acid orange, using an organo- silica binder and enhancing its activity by different curing methods (curing by UV-3h shown the best activity).

Appropriate techniques of structural characterization of a model hydrogel system

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Semi-interpenetrating polymer networks represent a unique way to modulate chemical and morphological properties of hydrogels and thus to control their basic properties essential in their practical applications (cosmetics, drug delivery systems, etc.). For this reason, it is crucial to analyze and describe the structure of the hydrogel correctly.

The main focus of this work was testing the applicability of available structural analysis techniques on an appropriate model hydrogel system and assessing the influence of the composition change of the hydrogel system on its internal structure. Semi-interpenetrating network hydrogels based on combination of agarose and sodium poly(styrene sulfonate) of various concentrations were chosen as a model system. Reference gels of four agarose concentrations were studied (0.5 %; 1.0 %; 2.0 % and 4.0 %) and compared with the gels with fixed concentration of agarose (1 wt. %) interpenetrated by polystyrene sulfonate at various concentrations (0.002 %; 0.005 % and 0.01 %). Swelled (hydrated) forms of the gels are usually used for applications, so it is convenient to examine samples in this state; however, there are not many common and available methods suitable for examining the structure of hydrated samples. Dry samples show artifacts in their structure due to eliminating water, e.g. structure of freeze-dried samples is affected by water freezing and subsequent crystal growth. By optimizing the drying process, this effect can be minimized. For dry (shock-frozen in liquid nitrogen and vacuum freeze-dried) samples, mercury porosimetry as an indirect method and scanning electron microscopy (SEM) as a direct method were selected in this study. For native (swelled) samples, turbidimetry as an indirect method and cryo SEM as a direct method were performed.

Cryo-SEM provided detailed and realistic visualization of the internal structure for the native samples (the pores scale down with increasing concentration of agarose). Dry samples (visualized by SEM) exposed pores slightly larger (the difference in hundreds of nanometers) than the native samples observed by cryo-SEM probably due to greater effect of emerging water crystals. Cryo SEM and turbidimetry provided comparable results of pore diameters (hundreds of nanometers). Mercury porosimetry has proven to be a suitable method only for the determination of

larger pores, in the case of small pores, the structure has already been destroyed by high applied pressures.

Keywords: hydrogel, structural analysis, electron microscopy, mercury porosimetry, turbidimetry

The Novel Materials for Bioelectronic Devices and Sensors

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Organic bioelectronics presents a potential revolution in disease treatment. Its function is based on the stimulation of biological tissues or reversible transmission of biological signals to the electrical ones. Therefore, these devices hold the promise of personalized treatment with reduced side effects compared to conventional pharmaceutical drugs. Conducting polymers have emerged as an excellent tool for the construction of these devices, especially due to their unique combination of electronic and ionic conductivity properties. One of the most promising conductive polymers in this field is polythiophene derivative poly(3,4-ethylenedioxythiophene) (PEDOT), particularly in the form with poly(styrene sulfonate) anions (PSS) as counterions (PEDOT:PSS). This material possesses excellent conductivity and chemical stability. However, its biocompatibility is only limited, which is the main drawback of this polymer, as the proper connection of the device with the living organism is one of the crucial requirements for the convenient function of the devices and thus for the successful treatment.

The presented work is focused on the characterization of the novel materials based on the PEDOT molecule that would offer improved biocompatibility and hydrophilicity compared to the polymer PEDOT:PSS. For this purpose, two approaches are being utilized. The first approach is to modify the surface of PEDOT:PSS with a biocompatible molecule. Therefore, a novel technique for modification of PEDOT:PSS surface by the arginine-glycine-aspartic acid (RGD), using a bifunctional photolinker sulfo-SANPAH was studied. Using different methods, the conjugation of the RGD peptide to the polymer surface was confirmed. Subsequently, the biocompatibility assay showed this process led to the improved biocompatibility compared to the original PEDOT:PSS.

Moreover, the material with dodecylbenzene sulfonate acid (DBSA) used as a counterion (PEDOT:DBSA) was investigated as the limited biocompatibility of PEDOT:PSS is most likely due to the presence of cell adhesion-restricting sulfonate groups of PSS moiety. This material proved to have improved biocompatibility compared to PEDOT:PSS. The viability of cells grown on PEDOT:DBSA is twice as high as those grown on PEDOT:PSS. Furthermore, in order to improve the long-term stability and hence the long-term biocompatibility of PEDOT:DBSA, the

crosslink of this material using a crosslinking agent GOPS ((3-glycidyloxypropyl) trimethoxysilane) was performed. Using different methods, it was confirmed the crosslink of the material was successful. Subsequently, the delamination test showed significant improvement of the resistance against the delamination as well as against dissolution of the thin film of the material.

Pilot gas scrubber and its efficiency

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This work deals with separation of pollutant gasesous and solid particles from air mass, which arise during combustion of fossil fuels from various industrial sources, but also during combustion of common fuels in households or emissions from automobile exhaust gasses. In all these cases, this is mainly a problem of greenhouse gases where CO2 accounts for the largest share-separation using a device can very well separate harmful solid particles and harmful gaseous substances from the air. In these devices the is a process called absorption. Polluted gas is sucked into the scrub head by suction and liquid is sprayed against this polluted gas as soon as the two phases (liquid and gaseous) come into contact with process called absorption. In our laboratory, we dealt specifically with the issue of CO2 separation using 1% NaOH solution. It was measured at different flow parameters of CO2 gas and at various flow parameters of a liquid with 1% sodium hydroxide solution. It was also very necessary to select a suitable nozzle for measurement, since different types of nozzles create different types of droplets, which also affect the separation efficiency. The gas scrubber achieved an efficiency of up to about 70% separation of CO2 gas from the air. In the next steps, we looked at improving the efficiency of separation, so it is planned to install multiple nozzles for the gas scrubber.

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Keywords: gas scrubber, liquid, gas, carbon dioxide, sodium hydroxide, efficiency, absorption,