Studentská odborná konference
Chemie je život 2022

Sborník abstraktů

Vysoké učení technické v Brně

Fakulta chemická, 30. listopadu 2022

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DNA-vazebné proteiny v interakci se strukturou guaninového kvadruplexu

Adéla Adamová

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ada.adamova@email.cz

Molekula DNA je nejvíce známá jako dvouřetězcová pravotočivá šroubovice. Za některých podmínek se objevují i nestandartní sekundární uspořádání jako jsou například čtyřřetězcové guaninové kvadruplexy, které zkoumám této práce. Vyskytují se v oblastech bohatých na guanin. V lidském genomu je přes 700 000 oblastí, které jsou výhodné k jejich tvorbě. Jsou to ve velké většině regulační oblasti nebo konce chromozomů. Sekundární struktury představují vhodné cíle pro vazbu velkého množství proteinů, které obsahují strukturní motivy důležité pro tuto interakci. V tomto projektu bude pomocí biochemických, biofyzikálních a molekulárně biologických metod zaměřena pozornost na vazebné motivy zinkového prstu a RGG boxu různých proteinů ve vztahu k DNA v různých konformacích.

Poděkování

Chtěla bych zejména poděkovat mému školiteli Mgr. Denisovi Šubertovi, za to že mi dal šanci pracovat na odborném pracovišti, čímž jsem měla tu možnost si rozšířit obzory v tomto oboru. A celkově i sympatickému a přátelskému prostředí, který Biofyzikální ústav poskytuje.

Dále bych chtěla poděkovat Mgr. Haně Holubové za pomoc, jako školní konzultant, a také celkově SPŠ Chemické, že umožňuje nám studentům se zúčastnit takových projektů, které nás mnohdy mohou motivovat na navazující studium.

A nakonec bych chtěla poděkovat JCMM za průběžné a přehledné informování ohledně prací SOČ.

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Chemická modifikace 2D MXenů

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Práce pojednává o dosud nepopsaných 2D karbidech přechodných kovů, tzv. MXenech, konkrétně o moderní skupině modifikací karbidu molybdenu a jejich izomerů, které jsem vybral na základě vlastní rešerše vědeckých článků. V dostupné literatuře jsou zcela nepopsané až na dvě výjimky, které jsou ovšem neadekvátní. Elektrické a optické vlastnosti jsem studoval na nejvyšší možné úrovni, kterou mé schopni a možnosti dovolily, protože jsem na základě dostupných informací předpokládal jejich potenciál ve fotovoltaice. Pomocí přesných výpočtů jsem určil, zdali se jedná o elektricky vodivé, či nevodivé materiály a zdali absorbují vlnové délky viditelného světla. Ústřední výstupy mé práce jsou hodnoty zakázaných pásů a absorbance viditelného světla. Zakázaný pás jsem na počátku zkoumání určil díky teorie funkcionálu hustoty (Density-functional theory, DFT), přesněji jednoduché metody Perdew-Burke-Ernzerhof, tzv. PBE, poté přesnější hybridní metody, tzv. HSE06, a na závěr nejexaktnější mnohočásticové poruchové metody GW. Optické vlastnosti jsem počítal pomocí Bethe-Salpeterovy rovnice (BSE).

Výsledky práce lze kategorizovat do dvou skupin – základní výzkum a aplikovatelný. V rámci základního výzkumu jsem obohatil vědeckou komunitu o hodnoty mřížkových konstant u všech materiálů a izomerů, které nebyly doposud exaktně stanoveny, ale jsou naprosto klíčové pro všechny výpočty. Vypočítal a porovnal jsem celkové energie materiálů i jejich izomerů, čímž jsem deklaroval, která forma má vyšší pravděpodobnost existence. Zjistil jsem, že izomery jsou vždy energeticky nevýhodné – řádově o několik jednotek eV – a jsou elektrické vodiče s takřka nulovým zakázaným pásem.

Druhým odvětvím bádání byly optické vlastnosti, které nebyly v dostupné literatuře žádným způsobem popsány. Pomocí metody BSE jsem určil vazebnou energii excitonů a energii zakázaného optického pásu. Vyvodil jsem praktické aplikace pramenící z perspektivních optických a elektrických vlastností. Patrně největší přínos své práce vidím v možném ulehčení ekonomické náročnosti, protože náklady na experimenty jsou zatěžující, a provedené výpočty šetří finance i čas a jsou nanejvýš průkazné. Práce odpovídá otázkám na všech úrovních ohledně elektrických a optických vlastností. Se znalostí zakázaného pásu je možné přesně určit, o jak dobrý elektrický vodič, polovodič či izolant se jedná.

Nejvýraznějším materiálem je karbid Mo2CF2, který svým nepřímým zakázaným pásem připomíná křemík a jeho monoatomární vrstvy pohlcují až 12 % dopadajícího světla, čímž předčil křemík. Na základě těchto dvou faktorů je materiál velmi perspektivní pro využití ve fotovoltaických článcích. Další materiály Mo2CCl2 a Mo2C(OH) 2 odpovídají klasickým polovodičům a jsou schopné absorbovat až 10 % dopadajícího světla, čímž pouze lehce zaostávají za dominujícím Mo2CF2. I přesto, že v mé práci nenabízejí špičkové vlastnosti, v porovnání s konvenčními materiály jsou nadprůměrné. Výjimku v rámci mého bádání tvoří Mo2CO2, který měl jiné technické parametry, ale hlavně je jako jediný vodič. Díky tomu, že jeho

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Motivací práce bylo, ať přispěje k rozvoji základního výzkumu 2D světa, pomůže pokračovatelům – dalším studentům a vědcům – a nabídne cenné podněty a lákavé alternativy pro svět průmyslu. V neposlední řadě si přeji, ať slouží k osvětě dvoudimenzionálních materiálů, protože se jedná o nádherný svět.

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Pesticidy v ovoci a zelenině

Petra Janíčková

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Práce se zabývá zjištěním obsahu pesticidů ve zvoleném ovoci a zelenině pomocí vysokoúčinné kapalinové chromatografie (UHPLC) spojené s detekcí pomocí hmotnostní spektrometrie s vysokým rozlišením (HRMS). Zvolený postup bylo možné provést pouze se vzorky s vyšším obsahem vody jak 70 % a obsahem tuku nižším jak 10 %. Vzorky ovoce a zeleniny byly ze stromu (meruňky), keře (rajčata) a ze země (jahody). Každý druh ovoce a zeleniny byl pořízen ze čtyř zdrojů: domácí ovoce a zelenina, BIO ovoce a zelenina, ovoce a zelenina z tržnice a koupené ovoce a zelenina v běžném supermarketu v ČR. Cílem bylo porovnat mezi sebou naměřené koncentrace pesticidů a různé zdroje produktů. Též vytvořit stručný přehled používaných pesticidů v dnešní době a jejich stručná charakteristika.

Pesticidy v ovoci a zelenině

Petra Janíčková

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Zjišťování těžkých kovů uvolňovaných z armatur do pitné vody

Jan Jirků

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Tato práce se zabývá problematikou čistoty vody a potrubním systémem, ze kterého se mohou uvolňovat nebezpečné látky jako těžké kovy. Zaměřuje se převážně na vliv těchto látek na člověka, jejich biochemické vlastnosti, vliv na prostředí a na legislativu spojenou s tématikou čistoty vody. Také popisuje analytickou metodu spektrofotometrie, která byla využita v praktické části. Praktická část obsahuje popis tvorby a analýzy výluhových vzorků 7 druhů potrubí. Naměřené hodnoty jsou nakonec porovnány s limity stanovenými legislativou.

Výsledky práce upozorňují převážně na nebezpečí používání starých nevhodných druhů potrubí, jako je například pozinkované potrubí, a na jiná nebezpečí, která mohou přicházet s pitím vody z vodovodního potrubí.

Poděkování

Chtěl bych poděkovat panu Ing. Buriánkovi za pomoc s touto prací. Také bych chtěl poděkovat panu Ing. Jungovi a paní Ing. Machů z Mendelovi univerzity za jedinečnou příležitost práce na tomto tématu. Nakonec bych chtěl poděkovat JCMM za možnost vypracovat tuto práci a za finanční podporu.

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Jedlé biodegradovatelné obaly

Tomáš Nerád

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Tato práce pojednává o jedlých biodegradovatelných obalech. Teoretická část je zaměřena v první řadě na druhy jedlých obalů, možná využívaná aditiva a možnosti aplikace těchto obalů v praxi. Dále se rozebírají témata jako je například kompostování, antokyany či balení výrobků do různých druhů obalů v závislosti na konzistenci výrobku. V části práce se také porovnávají výhody a nevýhody jednotlivých biodegradovatelných obalů. Experimentální část je založena na zkoumání vlastností více druhů vyrobených obalů v závislosti na odlišných okolních podmínkách. Dále jsou za účelem přiblížení fyzikálních a chemických vlastností obalů, na bázi κ-karagenanu, využity různé metody. Ty zahrnují zkoumání nejdůležitějších požadavků na obaly, jako například tloušťku, pevnost, flexibilitu a stanovení celkového počtu polyfenolů. V závěru byla z naměřených výsledků zpracována data a vyhodnoceny statisticky významné rozdíly mezi jednotlivými měřeními.

KLÍČOVÁ SLOVA
Obal; biodegradace; antioxidační aktivita; karagenan

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Obal; biodegradace; antioxidační aktivita; karagenan

Syntéza molekulárních prekurzorů a jejich aplikace v syntéze nanočástic slitin kovů

Michael Sedláček

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Nanotechnologie je v posledních několika desetiletích rapidně se rozvíjejícím oborem s nedozírným potenciálem. Vědci po celé Zemi dnes usilovně pracují na prohlubování znalostí o světě na nano-škále. Nanotechnologie nachází širokou řadu uplatnění, např. v medicíně, elektrotechnickém průmyslu, stavebnictví a v dalších oborech, její rozvoj je tedy pro benefit nás všech i lidí dobudoucna.

Jeden z přístupů, který lze k rozvoji nanotechnologie pojmout, je její manipulace skrz syntézu nanočástic s konkrétními požadovanými vlastnostmi. Tato práce se zabývá právě vlivem, který mají výchozí látky na výsledné nanočástice. Práce si klade za cíl syntetizovat nové prekurzory obsahující stříbro, charakterizovat je a následně je použít pro přípravu nanočástic slitiny AgCu, taktéž je popsat, a sledovat vliv, jaký na ně měl použitý prekurzor.

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Histologická separace vrstev kůže při fixaci těla a její využití ve forenzní daktyloskopii

Lucie Sedlaříková

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Tato práce se zabývá histologickou separací vrstev kůže na bříšcích prstů při fixaci těl lihovou metodou.

Moje studie volně navazuje na studii mé konzultantky paní doktorky Dzetkuličové. Paní doktorka Dzetkuličová vypracovala studii ohledně oddělování jednotlivých kožních vrstev na fixovaných lidských tělech za pomocí fixační techniky podle anatoma Waltera Thieleho. Moje práce navazuje na její práci tak, že také pozoruji danou problematiku, jen v menším časovém měřítku a s tím rozdílem, že v mé práci jsou těla fixovaná lihovou metodou.

Cílem práce je pozorovat a popsat oddělení jednotlivých vrstev kůže třecího hřebene na bříšcích prstů. Dalším cílem je zjistit, zda dochází ke kompletnímu oddělení epidermis od dermis. Také chceme zjistit, zda je lihová metoda vhodná pro pozorování oddělování jednotlivých vrstev, aby bylo možné zkoumat a srovnávat dermální otisky prstů s epidermálními otisky. Získání „modelu“ pro možné srovnávání epidermálních a dermálních otisků prstů je potřebné pro trénink forenzních daktyloskopů a další výzkum.

Tato práce popisuje postupné odběry vzorků kůže v oblasti třecího hřebene prstu na ruce u dvanácti jedinců a pozorování oddělování jednotlivých vrstev v čase před fixací těla až čtvrtý týden po fixaci těla lihovou metodou.

V praxi tento výzkum bude užitečný v případech, když v důsledku rozkladných procesů bude na neznámém mrtvém těle chybět vrstva epidermis na bříšcích prstů. Aby bylo v takovém případě možné identifikovat lidské tělo, bude potřeba porovnat posmrtné dermální otisky prstů s epidermálními otisky, které byly odebrány před smrtí jedince. Jelikož je takových případů ve forenzní praxi minimum, experti se nestřetají s dostatečnými prostorem jak pro nácvik odběru dermálních otisků prstů z těl, tak i pro porovnání dermálních a epidermálních otisků prstů. Proto je tedy důležité získat ,,modely“ pro srovnání obou otisků.

Klíčová slova: dermis; epidermis; fixace těla; oddělení vrstev kůže; stratum corneum; stratum lucidum

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Klíčová slova: dermis; epidermis; fixace těla; oddělení vrstev kůže; stratum corneum; stratum lucidum

Funkce cyklin-dependentní kinázy 13 v buněčné signalizaci

Emma Šilhavá, Tomáš Frybert

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Tématem naší práce je funkce cyklin-dependentní kinázy 13 v buněčné signalizaci. V teoretické části se zabýváme základy buněčného dělení. Dále se zabýváme popisem transkripce, RNAPII a následně samotnou CDK. V praktické části využíváme metodu western blot, která je klíčovou metodou pro naši práci. Sledujeme vliv deplece proteinu CDK13 na různé myší embrya ve stádiu E12,5 dne. Tyto změny pozorujeme v buněčných drahách Reelin a Hemogen.

Poděkování

V první řade bychom chtěli nejvíce poděkovat Mgr. Jiřímu Kohoutkovi, Ph.D. za ochotu, trpělivý přístup a vedení SOČ. Dále také za poskytnutí vzorku a prostoru laboratoří na Masarykově univerzitě. Další díky patří Mgr. Haně Holubové, která byla naším školním konzultantem, a Mgr. Tomáši Buriánkovi za poskytnutí veškerých informací ohledně vypracování práce.

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Studium chemických reakcí probíhajících při pražení kávy

Michaela Štěpánková[1], Denisa Frýbortová[1], Pavel Diviš[2]

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Zelená káva se získává z plodů kávovníku, který roste v subtropickém a tropickém, tzv. kávovém pásmu. Samotná zelená káva není poživatelná. Teprve pražením nabývá kávové zrno charakteristických vlastností. Pražení představuje nejdůležitější fázi při úpravě kávy. Nevhodným upražením lze i nejkvalitnější kávu úplně znehodnotit a správným postupem naopak levnější sortu podstatně zlepšit.

Cílem naší práce bylo sledování změn chemického složení kávového zrna při pražení kávy. Pro experiment jsme použily kávu Brazil Cerado dulce a tuto kávu jsme pražily v domácí pražičce při teplotě 220 °C celkem 15 minut. Během pražení jsme z pražičky postupně v časových intervalech odebíraly vzorky pražené kávy a ty jsme pak analyzovaly. Sledovaly jsme obsah sacharidů, organických kyselin a fenolických látek metodami vysoko-účinné kapalinové chromatografie, iontové chromatografie a molekulové absorpční spektrometrie. Pro extrakci sledovaných látek z kávového zrna jsme použily směs ethanolu a vody a magnetickou míchačku.

Výsledky práce ukázaly, že nejvíce zastoupeným sacharidem v kávovém zrnu je sacharóza, která během pražení postupně degraduje, čímž vznikají organické kyseliny, především kyselina octová a kyselina mravenčí Množství celkových fenolických látek se v kávovém zrnu během pražení příliš nemění a pravděpodobně pouze dochází k přeměně těchto látek na jiné aktivní látky, například pyrogallol apod.

Studium chemických reakcí probíhajících při pražení kávy

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Výsledky práce ukázaly, že nejvíce zastoupeným sacharidem v kávovém zrnu je sacharóza, která během pražení postupně degraduje, čímž vznikají organické kyseliny, především kyselina octová a kyselina mravenčí Množství celkových fenolických látek se v kávovém zrnu během pražení příliš nemění a pravděpodobně pouze dochází k přeměně těchto látek na jiné aktivní látky, například pyrogallol apod.

Stopové prvky ve stravě – mangan, měď, zinek

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Na naší planetě nám neustále roste populace a s ní se zvyšují požadavky na produkci potřebných potravin. Jelikož orná plocha je omezená, tudíž je tato produkce omezená a plocha se musí používat opakovaně, což může vést k absenci nezbytných prvků pro lidský organismus v těchto potravinách. Mezi tyto prvky můžeme zařazovat minerály, vitamíny a primárně stopové prvky.

Stopové prvky jsou chemické prvky, které náš organismus potřebuje v malém množství ke správnému vývoji. Zároveň tyto prvky nemohou být v těle samy vytvářeny a musejí být přijímány potravou. Jejich dlouhodobá absence proto může mít pro organismus velmi nebezpečné důsledky. Z tohoto důvodu jsou v dnešní době stopové prvky do potravy přidávány uměle. Zde ale může hrozit druhé riziko a tím je toxicita. Toxicita stopovým prvkem je jeho dlouhodobé nadměrné požívaní. Tato toxicita je pro organismus opět velmi nebezpečná. Důsledkem toxicity či deficitu stopových prvků může být selhání jater, poškození mozku nebo i smrt organismu.

Tato práce je zaměřená na stopové prvky mangan, měď a zinek. Cílem práce je vytvoření přehledu pro každý z prvků po stránce funkcí v organismu, po stránce důsledků deficitu či toxicity a po stránce procesu vstřebání prvku do organismu. Dalším cílem práce je stanovení těchto stopových prvků v doplňcích stravy za použití metody plamenové atomové absorpční spektrometrie (F–AAS). Pro mangan byl použit doplněk stravy Man Energy 30+ značky Pharmaton, pro měď byl použit doplněk stravy Pharma Activ a pro zinek byly využity doplňky stravy zinku GymBeam a Allnature.

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Sekce studentů bakalářských a magisterských studijních programů

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Príprava a charakterizácia nových typov selektívnych kompozitných membrán na báze polyméru Pebax a nanočastíc MOF UiO-66-NH_2

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Problematika efektívneho zachytávania a odstraňovania CO2 zo zmesi plynnou predstavuje zásadný príspevok k zmierňovaniu klimatickej zmeny. Zníženie emisií CO2 pomocou membránových technológií sa v porovnaní s inými technikami považuje za čisté a nákladovo efektívne. V priebehu posledných 20 rokov sa materiálový výskum zameral na vývoj zmiešaných matricových membrán (MMM), ktoré obsahujú anorganické nanočastice v polymérnej matrici. Novo vynájdené MMM materiály vykazujú lepšie mechanické a aj separačné vlastnosti oproti neplneným polymérom. V tejto práci bol ako polymérna matrica v MMM použitý Pebax, ktorý obsahuje tuhé polyamidové (PA) a flexibilné polyéterové (PEO) segmenty so zvýšenou afinitou voči CO2. Do MMM boli zabudované kovo-organické nanočastice MOF (UiO-66-NH2), ktoré poskytujú dusíkové atómy ako väzbové miesta pre molekuly CO2. Pridanie MOF nanočastíc do matrice membrány spôsobilo významné zvýšenie permeability a selektivity u dvojíc plynov CO2/N2, CO2/CH4, CO2/H2 a O2/N2. Už len u membrány s 5 hm. % zastúpením MOF nanočastíc sa selektivita CO2/N2 zvýšila z hodnoty 45 na hodnotu 51 v porovnaní s čistým Pebaxom, pričom sa prekonala Robesonova horná hranica (2008). U membrány s 10 hm. % UiO-66-NH2 sa priepustnosť oxidu uhličitého taktiež zvýšila o necelých 34 % aj s nárastom selektivity CO2/N2. Kombinácia Pebax-MOF sa javí ako potenciálna použiteľná pre aplikácie pre separácie plynov, napr. na zachytávanie a ukladanie CO2.

Morfológia membrán a ich chemické zloženie boli skúmané analytickými metódami: ATR-FTIR, XRD, 3D optickým profilometrom, SEM a SEM-EDS analýzou.

Príprava a charakterizácia nových typov selektívnych kompozitných membrán na báze polyméru Pebax a nanočastíc MOF UiO-66-NH_2

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Akcelerace mikrobiologických výzkumů za využití strojového učení

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Pěstování mikrobiálních kultur na kultivačních médiích je metodou, přirozeného nárůstu populace mikroorganizmů za kontrolovaných laboratorních podmínek, sloužící k jejich identifikaci, či ke zkoumání efektu vnějšího prostředí na jejich intenzitu reprodukce v čase. V současné době jsou tyto experimenty velice rozšířené, čímž dochází ke stále větší potřebě efektivních kvantitativních a kvalitativních vyhodnocovacích metod.

K vyhodnocování mikrobiálních kultur se obvykle využívá softwarů, které nedokáží z fotografií kultur samostatně vyhodnotit zastoupení mikromycet, a je tak potřeba manuální asistence pracovníka u každé z fotografií, což je značně neefektivní, nepřesné a nespolehlivé, což doposud značně omezovalo výzkumnou činnost v této oblasti.

Aurora za využití strojového učení dokáže nejenom s vysokou přesností klasifikovat jednotlivé zóny a získat tak jejich relativní velikost v daném čase ale i spočítat počet kolonií a z kombinace těchto dat získat distribuci relativní velikosti jednotlivých kolonií, což je úplně novou metodou, která by mohla poodkrýt nových souvislostí v prováděných experimentech, a to vše takřka bez nutnosti uživatelského vstupu, čímž se celý proces vyhodnocování v podstatě kompletně automatizuje, což vede k masivnímu zrychlení, díky čemuž je možné provádět rozsáhlejší experimenty s kvalitnější statistikou a tak i podstatnějšími výsledky.

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Antioxidační aktivita ligninových nanočástic

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Lignin je společně s celulózou a hemicelulózou přítomen v sekundárních buněčných stěnách rostlin. Z chemického hlediska má lignin amorfní a vysoce rozvětvenou strukturou s širokým obsahem funkčních skupin. Tyto skupiny jsou zodpovědné za jeho jedinečné vlastnosti, mezi které se řadí absorpce UV záření, antimikrobiální nebo antioxidační aktivita. Zároveň je lignin také považován za nejrozšířenější aromatický biopolymer na Zemi. Navzdory velkému potenciálu využití, je jedna z hlavních překážek skutečnost, že lignin izolovaný z různých zdrojů a různými metodami, disponuje odlišnou strukturou a vlastnostmi. Efektivního využití ligninu lze dosáhnout snížením velikosti částic na nanorozměry. Tyto nanočástice mohou najít uplatnění v různých aplikacích, jako jsou nosiče léčiv, antikorozní výplně kovů a antioxidační nanokomponenty s ochranou proti UV záření.

Tato práce se zaměřuje na přípravu nanočástic s vysokou antioxidační aktivitou z komerčně dostupného kraft ligninu. Nanočástice byly připraveny metodou solvent-exchange, přičemž byla porovnána různá rozpouštědla ligninu s důrazem na nízkou toxicitu. (např. voda, methanol, dimethylsulfoxid). U získaných nanočástic byla stanovena antioxidační aktivita metodou zhášení radikálů kyseliny 2,2‘ azino bis(3 ethylbenzothiazolin-6-sulfonové)) (ABTS). Velikost a stabilita získaných nanočástic byla analyzována pomocí dynamického a elektroforetického rozptylu světla. Na základě provedených měření byla potvrzena vysoká antioxidační aktivita a pomocí vody a dimethylsulfoxidu se podařilo připravit nanočástice v rozměrech 45–100 nm. Tato práce poukazuje na skutečnost, že přípravou nanoligninu se významně rozšiřují aplikační možnosti ligninu v různých odvětvích průmyslu. Aplikace nanočástic jako plniva pro hydrogely bude předmětem naší další práce.

Poděkování:
Táto práce byla podpořena interním grantem FCH VUT (FCH-S-22-7909).

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Riadené uvoľňovanie liečiv z magnetolipozómov

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V súčasnosti je drvivá väčšina liečiv podávaná pacientom systémovo, kedy prítomnosť účinných látok v celom organizme podmieňuje ich potrebné vyššie dávky a zároveň možné vedľajšie účinky. Túto skutočnosť sa usiluje zmeniť koncept cieleného doručovania a riadeného uvoľňovania liečiv, realizovateľný prostredníctvom rôznych nosičov, ktoré by mohli priniesť zdravotné (minimalizácia nežiadúcich účinkov) aj ekonomické (minimalizácia potrebnej dávky) benefity. Ako vysoko potenciálne nosiče sú predstavované magnetolipozómy, submikrónové kompozity, kombinujúce magnetické nanočastice s lipozómami. Okrem signifikantných transportných vlastností vykazujú vďaka svojim fyzikálnym vlastnostiam superparamagnetizmus, ktorý otvára možnosti využitia rádiofrekvenčného (RF) poľa na riadené uvoľnenie liečiv.

Práca v prvej časti študuje vlastnú prípravu magnetolipozómov, ich základné parametre a vlastnosti. Magnetické nanočastice, stabilizované fosfolipidovým obalom, boli opakovateľne pripravené modifikovanou koprecipitačnou metódou dosahujúc veľkosť jadier 6±1 nm (obrazová analýza z TEM). Magnetolipozómy boli opakovateľne pripravené metódou hydratácie lipidového filmu s prídavkom magnetických nanočastíc použitím fosfátového tlmiču (PBS) (Obr. 1). Na ohraničenie maximálnej veľkosti bola využitá extrúzia cez polykarbonátové membrány so špecifickými veľkosťami pórov. Vzorky magnetolipozómov vykazovali aj po extrúzii polydisperznú distribúciu veľkostí častíc, upraviteľnú magnetickou separáciou. Koncentrácia železa vo vzorkách bola spektrofotometricky určená v rozmedzí 0,1 – 0,3 mg železa/mg fosfolipidov. V stacionárnom magnetickom poli (B = 87±9 mT) dosahovali podľa obrazovej analýzy jednotlivé kompozity rýchlosť pohybu až 50 μm/s (približne 120-násobok ich vlastnej dĺžky za sekundu). Experiment v laminárnom prúdení, modelujúci ľudské vlásočnice, ukázal schopnosť magnetolipozómov vytvoriť ustálený film na stene kapiláry. Pri optimálnom zložení lipozomálnych membrán – dipalmitoylfosfatidylcholín, dimyristoylglycerofosfát sodný a cholesterol – bola magnetolipozómom v RF poli nameraná priemerná rýchlosť ohrevu 0,38 °C/s (SAR ≈ 600 W/g).

Práca ďalej diskutuje správanie magnetolipozómov s modelovou liečivou látkou, norfloxacínom (NFX). Nosiče s obsahom antibiotika NFX boli analogicky pripravené hydratáciou NFX roztokom v PBS. Prítomnosť NFX v magnetolipozómoch bola potvrdená extrakciou do metanolu. Norfloxacín sa podarilo vylúčiť aj pôsobením RF poľa, pričom časovo dlhšie vystavenie a vyššie dosiahnuté teploty viedli k väčšiemu množstvu uvoľnenej látky. Uvoľnenie NFX bolo sledované v RF poli aj pri fyziologických teplotách, avšak vystavenie magnetolipozómov externému zdroju zahrievania pri rovnakej teplote k tomuto efektu neviedlo. Na základe

Riadené uvoľňovanie liečiv z magnetolipozómov

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Mikroreologické modelování nástrojem COMSOL Multiphysics

Jakub Koláček

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Studiu hydrogelů jako nosičů léčiv nebo sledování transportu léčiv v biologických systémech a tkáních je stále věnována větší a větší pozornost. Tyto systémy jsou charakteristické svou komplexností a studování jejich struktury a jak tato struktura ovlivňuje transport látek je pro tyto aplikace kritické. Pro řešení a studování této problematiky se právě využívají mikroreologické experimenty, zejména pasivní mikroreologie.

Poměrně novým přístupem na fakultě je využití simulací pro podporu těchto experimentů. Vzhledem k časové náročnosti klasických experimentů v laboratoři, ať už je to příprava vzorků nebo samotné měření, poskytují simulace jednoznačnou výhodu v rychlosti přípravy a vyhodnocení dat – při vhodně navržených modelech je možné simulacemi optimalizovat prováděné experimenty efektivněji a v mnohem kratším čase.

Cílem práce bylo navrhnout a vytvořit základní modely, které budou schopny věrně simulovat pohyb mikročástic ve viskózním a viskoelastickém prostředí a mohou být využity pro modelování pasivní mikroreologie. A dále rámcově poskytnout vhled do oblasti dalšího řešení této problematiky a otevřít tak cestu dalším simulačním experimentům.

Pro výpočet MSD z výsledků simulací byly vytvořeny skripty v programu Matlab a výsledné viskózní modely z této práce byly analyzovány jednoduchými studiemi a zároveň byla ověřena jejich shoda s experimentálními daty. Dále byly navrženy základní modely simulující viskoelastické prostředí, kde pro návrh těchto modelů byly zvoleny dva odlišné postupy, a to využití rigidních překážek za předpokladu diskrétního prostředí a matematický model uvažující kontinuální prostředí.

Výsledná data z viskózního modelu prokázala dobrou shodu s experimentálními výsledky a při modelování viskoelastického chování se nejvíce přiblížil kontinuální matematický model.

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Elektrochemické řízení oxidačního stavu homologů transaktinoidů

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Výzkum transaktinoidů, tedy prvků s protonovým číslem 104–121, se v posledních letech nezaměřuje již pouze na problematiku jejich syntézy a produkce, ale stále více i na analýzu jejich chemických charakteristik; mezi hlavní patří oxidační čísla, díky jejichž znalosti je pak možné předpovídat existenci z chemického hlediska stabilních sloučenin konkrétního transaktinoidu. Zároveň je důležité zjištění vlivu relativistických efektů, které se v těchto případech již významně projevují na jejich chování. Kromě nejrozšířenější thermochromatografie však lze také pro chemický výzkum těchto prvků využít metod elektrochemických.

Práce, jejíž dílčí výsledky jsou publikovány v rámci tohoto příspěvku, se věnuje počátkům návrhu průtokové elektrochemické aparatury (se zapojením potenciostatu Gamry Reference 600) pro provádění cyklické voltametrie za účelem zjištění oxidačního stavu homologů transaktinoidů, konkrétně india a thallia, tedy homologů nihonia (protonové číslo Z = 113) v roztocích o objemu nižších desítek mililitrů a při milimolárních koncentracích.

Poděkování

Poděkování patří docentu Mojmíru Němcovi, profesoru Janu Johnovi, doktoru Pavlu Bartlovi a doktorce Miroslavě Semelové za pomoc při provádění tohoto výzkumu. Práce byla ve své první půli realizována v rámci projektu „Development of a method for radiochemical separation and identification of neutron-rich isotopes of heavy elements produced in heavy ion nuclear reactions at single atoms level“, na kterém spolupracovala KJCH FJFI ČVUT a Flerov Laboratory of Nuclear Reactions / Joint Institute for Nuclear Research.

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Studium transportních a mechanických vlastností fyzikálních gellanových hydrogelů

Jan Sokolínský, Michal Kalina

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Hydrogely lze zjednodušeně představit jako zesíťovaná polymerní vlákna, která mezi svými řetězci poutají molekuly vody. Často toto množství vody výrazně převyšuje hmotnost nosné polymerní sítě hydrogelu. V současné době se výzkum zaměřuje na hydrogely, pro jejichž přípravu jsou využity polymery přírodního původu. V této práci byl pro přípravu hydrogelových systémů využit biopolymer gellan. Gellan je polysacharid, jehož produkce probíhá biotechnologicky za využití bakterie Sphingomonas elodea. V případě volby vhodného síťovacího činidla a aditiv využitých při přípravě gellanových hydrogelů jsou pak tyto materiály rovněž biokompatibilní a biodegradabilní, a jsou tak vhodnými kandidáty pro využití ve farmaceutickém průmyslu a medicínských aplikacích.

Hlavní náplní této práce bylo ověřit hypotézu, zdali je možné u fyzikálně síťovaných gellanových hydrogelů ovlivňovat transportní vlastnosti prostřednictvím cílené změny v postupu přípravy, resp. kompozice hydrogelové matrice. Ovlivnění transportních vlastností lze docílit dvojím způsobem. Prvním studovaným postupem byla změna koncentrace gellanu v kompozici hydrogelu, kdy tento způsob ovlivnění transportních vlastností byl studován na sadě vzorků o různé hmotnostní koncentraci biopolymeru v hydrogelu (1, 2 a 4 hm.%). Druhým využitým způsobem ovlivnění transportních vlastností byla změna iontové síly disperzního prostředí hydrogelu. Tento způsob byl studován na gellanových hydrogelech se 2 hm.% gellanu, kdy pro přípravu hydrogelu byla využita deionizovaná voda a 0,15 M roztok NaCl. Ke studiu transportních vlastností gellanových hydrogelů byl využit model difuzního páru, kdy byly dva hydrogely se stejnou hmotnostní koncentrací biopolymeru a shodným disperzním prostředím spojeny, jeden z hydrogelů navíc na počátku experimentu obsahoval konstantní koncentraci modelové sondy (methylenová modř) a takto připravený difuzní pár byl po definovaných časových intervalech měřen na UV–VIS spektrometru za využití posuvného držáku kyvety, umožňující zaznamenávat UV–VIS spektra v různé výšce v kyvetě. Za účelem lepšího porozumění, jaký vliv mají sledované modifikace postupu přípravy hydrogelu na jeho transportní vlastnosti, byly všechny studované hydrogely podrobeny charakterizaci základních viskoelastických charakteristik pomocí reometru HR–2 (TA–Instruments). V rámci reologické analýzy byly provedeny amplitudové oscilační testy. Ze získaných dat bylo zjištěno, že změnou koncentrace biopolymeru a vhodnou volbou disperzního prostředí lze modifikovat jak transportní, tak mechanické vlastnosti fyzikálních gellanových hydrogelů, což je výhodné pro potenciální aplikace, kde je nutné transportní charakteristiky definovaně řídit.

Studium transportních a mechanických vlastností fyzikálních gellanových hydrogelů

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Hydrogely lze zjednodušeně představit jako zesíťovaná polymerní vlákna, která mezi svými řetězci poutají molekuly vody. Často toto množství vody výrazně převyšuje hmotnost nosné polymerní sítě hydrogelu. V současné době se výzkum zaměřuje na hydrogely, pro jejichž přípravu jsou využity polymery přírodního původu. V této práci byl pro přípravu hydrogelových systémů využit biopolymer gellan. Gellan je polysacharid, jehož produkce probíhá biotechnologicky za využití bakterie Sphingomonas elodea. V případě volby vhodného síťovacího činidla a aditiv využitých při přípravě gellanových hydrogelů jsou pak tyto materiály rovněž biokompatibilní a biodegradabilní, a jsou tak vhodnými kandidáty pro využití ve farmaceutickém průmyslu a medicínských aplikacích.

Hlavní náplní této práce bylo ověřit hypotézu, zdali je možné u fyzikálně síťovaných gellanových hydrogelů ovlivňovat transportní vlastnosti prostřednictvím cílené změny v postupu přípravy, resp. kompozice hydrogelové matrice. Ovlivnění transportních vlastností lze docílit dvojím způsobem. Prvním studovaným postupem byla změna koncentrace gellanu v kompozici hydrogelu, kdy tento způsob ovlivnění transportních vlastností byl studován na sadě vzorků o různé hmotnostní koncentraci biopolymeru v hydrogelu (1, 2 a 4 hm.%). Druhým využitým způsobem ovlivnění transportních vlastností byla změna iontové síly disperzního prostředí hydrogelu. Tento způsob byl studován na gellanových hydrogelech se 2 hm.% gellanu, kdy pro přípravu hydrogelu byla využita deionizovaná voda a 0,15 M roztok NaCl. Ke studiu transportních vlastností gellanových hydrogelů byl využit model difuzního páru, kdy byly dva hydrogely se stejnou hmotnostní koncentrací biopolymeru a shodným disperzním prostředím spojeny, jeden z hydrogelů navíc na počátku experimentu obsahoval konstantní koncentraci modelové sondy (methylenová modř) a takto připravený difuzní pár byl po definovaných časových intervalech měřen na UV–VIS spektrometru za využití posuvného držáku kyvety, umožňující zaznamenávat UV–VIS spektra v různé výšce v kyvetě. Za účelem lepšího porozumění, jaký vliv mají sledované modifikace postupu přípravy hydrogelu na jeho transportní vlastnosti, byly všechny studované hydrogely podrobeny charakterizaci základních viskoelastických charakteristik pomocí reometru HR–2 (TA–Instruments). V rámci reologické analýzy byly provedeny amplitudové oscilační testy. Ze získaných dat bylo zjištěno, že změnou koncentrace biopolymeru a vhodnou volbou disperzního prostředí lze modifikovat jak transportní, tak mechanické vlastnosti fyzikálních gellanových hydrogelů, což je výhodné pro potenciální aplikace, kde je nutné transportní charakteristiky definovaně řídit.

Vývoj multifunkčních nanonosičů pro podávání léků

Markéta Štejdířová

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Biologicky odbouratelné polymerní nanočástice se často používají k ochraně molekul před degradací, pro zlepšení rozpustnosti léčiva, podpoře cílení léčiv a ke kontrolovanému uvolňování léčiva. Z různých biologicky odbouratelných polymerů, používaných jako nosiče pro dodávání léčiv a dalších molekul, je pravděpodobně nejpoužívanější kopolymer kyseliny glykolové a mléčné (PLGA).

Pro zlepšení protirakovinného terapeutického účinku chemoterapeutických léků a fotosenzibilizátorů je třeba navrhnout všestranné multifunkční nanoplatformy. K dosažení tohoto cíle byl v této práci vyvinut chemo-fototerapeutický lékový transportní systém založený na nanočásticích kopolymeru kyselin glykolové a mléčné (PLGA) a jeho analogech s polyethylenglykolem (PEG) koenkapsulací kolchicinu a purpurinu-18 (P18). P18 má velký potenciál jako protirakovinné léčivo používané ve fotodynamické terapii a jako činidlo pro zobrazování nádorů. Kolchicin je považován za antimitotikum, které zastavuje růst a proliferaci rakovinných buněk. Jejich společné zapouzdření do nanočástic může být nadějným přístupem k vybudování multifunkčního systému dodávání léků. Použití matrice PLGA nabízí snadné přizpůsobení povrchu a jedinečnou schopnost řízeného uvolňování. Pro dosažení cíleného dodávání byly v této práci navrženy, syntetizovány, charakterizovány a zhodnoceny nanonosiče PLGA konjugované s protilátkou pro cílené dodávání kolchicinu s P18 do buněk kolorektálního karcinomu a buněk rakoviny prsu.

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Zpracování koncentrátu z membránových procesů

Jan Vespalec
Martina Repková, Michaela Vašinová Galiová

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Jedna z hlavních denních potřeb lidstva je voda, a to voda o určité jakosti. Celosvětově je problém s kvalitou zdrojů vody. Alternativou k hledání zdrojů vody je použití vyčištěné odpadní vody jak pro účely pitné vody nebo pro účely užitkové vody. Vyčištěná odpadní voda je již dostatečně čistá a vhodná jako zdroj vody po řádném dočištění. K dočištění se ve většině případů používají membránové procesy. Produktem membránových procesů je kromě permeátu (voda o vhodné kvalitě) také koncentrát, který obsahuje zakoncentrované polutanty ze surové vody.

Cílem této práce je zmapovat možnosti likvidace koncentrátu jakožto odpadu. Pro likvidaci koncentrátu lze uvažovat o vypouštění do moře nebo kanalizace, dále zpracováním koncentrátu na odpařovacích rybnících nebo ve vakuových odparkách, další možností je recyklace solanky z koncentrátu nebo opětovné využití samotného koncentrátu. Při použití vakuové odparky je nutné nakládat s odpařeným koncentrátem obezřetně, neboť může být klasifikován jako nebezpečný odpad podle vyhlášky č. 8/2021 – katalog odpadů.

Poděkování:
Rád bych zde poděkoval firmě ASIO, spol. s r.o. za technickou podporu a spolupráci.

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Sekce studentů doktorských studijních programů

Tématický okruh vědy o živé přírodě a environmentální vědy

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Tématický okruh vědy o živé přírodě a environmentální vědy

Characterization of Biological Effects of Extracts Obtained from Yeasts

Jana Blažková[1], Dominika Špačková[2], Pavlína Sikorová[2], Pavlína Sniegoňová[2], Szotkowski Martin[2], Márová Ivana[2]

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Carotenogenic yeasts belong to the class Basidiomycota, which includes the following yeast genera: Cystofilobasidium, Rhodotorula and Sporobolomyces. All these genera are characterized by overproduction of carotenoids. If these genera have ideal conditions, they also produce high amounts of lipids. In addition, these lipids consist of fatty acids characterized by a high content of polyunsaturated and monounsaturated fatty acids, which find a wide range of uses in the food, pharmaceutical and agricultural industries. Therefore, carotenogenic yeasts are increasingly being investigated in the biotechnological industry.

The goal was to find out how carotenogenic yeast will behave in the presence of stress factors, and which of these stresses will have a positive effect on the production of metabolites that can be further used in various industries.

The experimental part dealt with the exposure of carotenogenic yeasts to oxidative stress and stress induced by heavy metals. The goal was to find out which concentrations of these stress factors are lethal for microorganisms, and which are optimal for increasing the production of the above-mentioned substances.

Of the yeast strains, Sporidiobolus pararoseus and Rhodotorula mucilaginosa strains achieved increased production of metabolites under the influence of selenate ions. Conversely, cobalt showed a favorable effect only on the accumulation of lipids in cells and β-glucans. However, the highest changes in metabolite production were achieved by addition of the optimal concentration of the oxidative stress-inducing solution.

Acknowledgement

The study was supported by the Internal grant competition, which is implemented as part of the OP VVV project entitled Quality internal grants BUT (KInG BUT); reg. number: CZ.02.2.69/0.0/0.0/19_073/0016948 specifically by KInG No. 7746

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Effect of Plasma Activated Water on Seed Germination

Ludmila Čechová, Tomáš Vozár, Kateřina Lišková, Kateřina Šindelková,
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One of the biggest concerns of modern agriculture is the contamination of agricultural soil and water by pesticides. The excessive use of pesticides might be affecting non-target organism such as aquatic organisms, birds, and animals. They can also have negative impact on human health.

Plasma activated water (PAW) is a new type of liquid fertilizer prepared by the interaction of plasma with liquids. The chemistry of plasma activated water is similar to the gas plasma chemistry, with short-lived reactive oxygen and nitrogen species (RONS) such as $\mathrm{NO}\cdot$, $\cdot\mathrm{OH}$ or $\cdot\mathrm{O2}-$. Subsequently, these short-lived species form long-lived RONS, such as hydrogen peroxide, nitrites and nitrates, which stay present in water for days. Thanks to $\mathrm{H2O2}$ and $\mathrm{NO2}-$, plasma activated water gains antibacterial properties, while $\mathrm{NO3}-$ serves as a source nitrogen and small amount of $\mathrm{H2O2}$ can stimulate germination and growth of plants. These properties can make plasma activated water a new and environmentally friendly tool to increase germination of seeds and subsequently, to increase and sustain agricultural production, while it may also protect the seeds from bacteria.

In this work, plasma activated water was prepared by three different plasma-liquid systems and it was characterized by measurements of pH, conductivity, and concentration of RONS. The first system was based on the dielectric barrier discharge in air with the liquid electrode. In the second system, plasma was generated directly in the liquid by high dc voltage, applied on the main pinhole-based electrode. In the third system, gaseous products from the dielectric barrier discharge were bubbled into the liquid. A mixture of oxygen and nitrogen (1:4) was used for plasma generation. Activation time was 2 minutes in all systems. The effect of plasma activated water on seed germination was tested on seeds of white mustard Sinapis alba, winter wheat Triticum aestivum and corn Zea mays.

Acknowledgement

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Sensor of food packaging environment quality

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The concept of intelligent food packaging is a modern approach on how to communicate information to the customer through packaging material. Indicators or sensors could indicate that the packaged food is still safe to consume past the use-by date or inform the consumer about the state of the modified atmosphere, implying possible food packaging rupture. This could potentially help to reduce food waste and ensure better food safety.

In this work an environment quality of food packaging sensor — an oxygen indicator – was studied. The oxygen indicator was based on photocatalytic reduction using microcrystalline titanium dioxide, redox dye, sacrificial electron donor and polymer matrix. The indicator gives a color change response to oxygen. The kinetics of the activation of the indicator and the color change were assessed from spectral measurements. The effect of sacrificial electron donor content on the kinetics of the reactions in the indicator was studied as well.

The oxygen indicator based on methylene blue is activated by UVA irradiation with intensity of only 0,1 mW·cm–2 in 48 s and the color change response in presence of oxygen is visible after 20 minutes. Further research in intelligent food packaging may include more comprehensive study of photocatalytic oxygen sensors, study of fluorescence-based oxygen sensors, indicators of ammonia, biogenic amines, or carbon dioxide.

Acknowledgement

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Problematic use of liquid chromatography for aminoclay-drug complexes

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This study aimed to use modern liquid chromatography for the evaluation of an aminoclay-drug complex and also to determine the amount of drug in this complex. The aminoclay-drug complex is a relatively new system for drug delivery in the human body. This connection was already studied by many types of analytical method with less or more successful results. The delivery matrix is based on organically modified aminoclay, magnesium phyllosilicate, which contains 3-aminopropyl groups. Because of these free groups, it is possible to have a binding molecule of the drug on the surface of complex. Aminoclay does not show signs of toxicity, and it has a very good chemical, mechanical, and thermal stability, and it is also highly soluble in water. These properties lead to the expectation in an increase of bioavailability of drug in the human body with the use of the aminoclay-drug complex instead of free drug or other drug carriers.

For verification of the binding drug, the method of liquid chromatography with less or more successful results depends on use chromatography system, columns and last but not least on type of binding drug. There exist many problematic parts of sample preparation and analysis, which can lead to a devaluation of results. One of the problems is the different solubility of the aminoclay matrix and drug in water. The mobile phase is based on water. Therefore, the solubility of pure aminoclay and aminoclay-drug is very high, but there is problem when the drug is insoluble in water. The main problem is that pure aminoclay could be invisible for liquid chromatography. Therefore, the use of liquid chromatography for the verification of the binding drug on the aminoclay matrix and especially its amount in the complex is very limitless and, in some cases, totally unusable as a direct method. In reference to that its open way to use liquid chromatography as indirect method how is descripted in this study.

Problematic use of liquid chromatography for aminoclay-drug complexes

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Heavy metal profiles in Antarctic lichens deciphered using solid sample instrumental probing microanalysis

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This presentation sums up efforts in a multi-instrumental environmentally focused approach to direct solid-sample chemical microanalysis with focus on trace metal accumulation in living systems. The effort aims to investigate the content and distribution of heavy metals of interest (Pb, Cd, Zn, Hg, Mn, Al, Cr, Cu) in thalli and hyphae of epilithic Antarctic fruticose lichens Usnea antarctica and U. auranticoatra from the James Ross Island and study their relationship with the surrounding environment and discuss bioaccumulating mechanisms and potential sources of heavy metal contamination in a clean, pristine environment. The influence of habitat and environmental conditions play an important role in the bioaccumulation of contaminants rather than simple presence of sources of contamination. A method for direct determination of metallic elements from lichen fungal tissue using LA-ICP-MS was developed for yielding optimal signal intensity during data acquisition using a state of the art 193 nm ArF laser (Elemental Scientific Instruments) hyphenated to a single collector sector field ICP mass spectrometer Element XR (Thermo Fisher). This presentation also introduces work in progress of methodical development of ToF-SIMS (TOFWERK, Thermo Fisher) analytical procedure as a comparative dimension of solid sample chemical microanalysis of trace metals in environmental samples.

Keywords: Antarctica, heavy metal, lichen, microanalysis, bioaccumulator, pollution, LA-ICP-MS, ToF-SIMS

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Poly(3-hydroxybutyrate) based materials for 3D printing in medical applications

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One of the most advanced approaches used in contemporary regenerative medicine is tissue engineering. The key role in tissue engineering is played by a porous structure (scaffold), which serves as a support for cells and is then integrated into the human body. The scaffold must have a suitable porosity and 3D structure for the cells to grow through the entire volume of it and form new tissue.

In recent years, a method of 3D printing is capturing attention in the bone tissue engineering field as it allows complex tailor-made structures to be produced in a time and cost-effective manner for every specific case and patient. Some bioplastics, such as polylactic acid, poly(3-hydroxybutyrate), or polycaprolactone are appealing not only for their environmental friendliness but also for their biocompatibility. [2] Recently, scaffolds from this group of polymers have been successfully produced. [3] Furthermore, tricalcium phosphate as well as hydroxyapatite can be used as a bioactive filler to promote in vivo osteogenic differentiation of mesenchymal stem cells.

The work focuses on research on 3D printing and testing of P3HB-based scaffolds for bone tissue engineering. Three polymer blends were prepared based on either commercial poly(3-hydroxybutyrate) or P3HB from the chloroform-free route, poly(lactic acid) and polycaprolactone, oligomeric adipate ester plasticizer, and tricalcium phosphate as a bioactive filler, and processed into the form of 3D printing filaments. The temperature tower test and warping test were conducted to determine the processing conditions for 3D printing. The lowest warping coefficient was 1.26 for a blend of poly(3-hydroxybutyrate) with polycaprolactone and plasticizer.

Tensile test, three-point flexural test, and compression test were used to study the mechanical properties of materials. Scaffolds with different surfaces were 3D printed from prepared filaments to determine the most optimal surface for cell proliferation. Optical contact angle measurement was conducted to determine the surface properties and their influence on cell adhesion, followed by the calculation of surface free energy. 3D printed surfaces were also subjected to roughness analysis by confocal microscopy to determine the effect of roughness on contact angle with water and cell growth. Finally, in vitro tests on scaffolds were conducted to classify the cytotoxicity of the materials and the influence of the scaffold´s surface on cell growth and proliferation.

In the end, two out of three materials were proven to be non-cytotoxic (both blends of poly(3-hydroxybutyrate) with polycaprolactone) and their mechanical

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Investigation of mercury removal from aqueous solution by wheat bran biochar using DGT technique

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The diffusive gradients in thin films technique (DGT) was developed in the 1970s for in situ analysis of natural systems. The principle of DGT technique is based on kinetic separation of chemical species from aquatic system according to Fick's First Law and their accumulation in sorption layer containing particles of specific adsorbent. The DGT technique has opened new possibilities in the analysis of microelements and organic residues, as the preconcentration in the sorption medium simultaneously separates the measured analytes from the matrix improving method detection limits. Traditional DGT devices employ sorption layer, diffuse layer and membrane filter enclosed in a plastic piston with cap. The diffusion and sorption layers consist of an agarose or polyacrylamide matrix, but the adsorption materials used for specific application have been the main focus of further development of DGT technique in recent years. One possibility is the use of waste materials from the food industry, which contains a lot of bioactive substances, or the pyrolysis of biological material into biochar, which has a significant adsorption capacity. For example, moringa seeds, spent coffee grounds or baker's yeast have already been used as adsorbents in DGT technique

This study focuses on characterization of adsorption properties of wheat bran pyrolyzed at 600 °C compared to mercapto-functionalized silica gel as a reference material. Agarose diffusive gels were prepared by casting of hot 1,5% agarose solution between two preheated glass plates separated by PTFE spacers having a thickness of 0,8 mm and left to cool at 4 °C. Binding gels were prepared by incorporating biochar with particle size below 200 μm into a 2% hot agarose gel using 0,5 mm PTFE spacers during suspension casting. Chemical composition and surface area of raw wheat bran, biochar and binding layer disks were characterized by Scanning electron microscopy, Energy dispersive X-ray spectrometry, ICP-OES spectrometry, IR spectrometry and BET isotherm. In order to study the uptake efficiency, binding kinetic, maximum adsorption capacity, effect of pH, ionic strength and another metal ions, agarose-biochar disks were placed in 40 ml of a 1 mg.l-1 mercury solution (0,01M NaNO3, pH 4,0±0,05; except monitoring influence of these parameters) under constant stirring for 24 hours in triplicate. The diffusion coefficients were determined by DGT time-series deployment method in 100 μg.l-1 mercury solution, the diffusion boundary layer (DBL) was determined by DGT deployment method using mercapto-functionalized silica binding gel in combination with diffusive layer with different thickness. This study has shown good adsorption potential of wheat bran biochar for mercury removal from aqueous solution without the presence of NaCl in pH range 3–7. Diffusion coefficient and maximum adsorption capacity of agarose-biochar binding gels were 6,24.10-6 cm2.s-1 and 0,50 mg.disk-1, respectively.

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Influence of Winery Wastewater Storage Period on its Processability in Wastewater Recycling Technology

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The winery wastewater (WWW) production is significant. The typical WWW amount is estimated at 1–4 l per 1 l of wine ; this sums to about tens of millions m3 in Europe. The WWW is produced mostly by equipment cleaning, during which compounds like ethanol, organic acids (mostly acetic acid), unfermented sugars, polyphenols etc. contaminate the WWW. Especially during vintage season (grape crushing), the WWW shows a high chemical oxygen consumption (COD) and low pH, which are extremely far from discharge limits to surface water, and typically not acceptable even for wastewater treatment plants. Also, the WWW composition is very inconsistent (COD values vary by up to three orders of magnitude with reported extremes of almost 300,000 mg/l). That is the reason why there is interest in development of WWW treatment and recycling technologies. The novel processes must be robust enough to handle WWW composition, while being economically viable and environmentally sustainable. A combination of evaporation and stripping showed promising results for COD reduction of WWW, and it also reflects the modern approaches to WWW. One such approach is Zero Liquid Discharge (ZLD), an idea of wastewater discharge elimination and a maximal recovery of water and other potentially valuable products. The published literature shows that the ZLD approach is yet to be applied to WWW, and there is also a limited amount of data about WWW composition. This lack of information creates a clear research gap, making the topic unique and suitable for further research. A solitary publication containing comprehensive analysis of a few WWW samples was used as a foundation for this research to identify important parameters and contaminants. WWW composition is crucial to assess the recycling technology's feasibility and aid the design procedure. The final set of parameters consists of COD, pH, amount of fructose, glucose, ethanol and acetic acid. WWW samples for this research were taken at winery in South Moravian region at the beginning of October 2022 (the critical period of the vintage season) and analyzed at biweekly (14 days) intervals for 1 month. Parameters were determined by different methods: COD photometrically using COD cell test, amount of fructose and glucose by HPLC, ethanol by GS–FID and acetic acid by IC. The COD value of 8310 mg/l was measured for the input sample and remain practically constant after 14 days and a month. The amount of sugars was already found to be negligible during the first analysis. The sugars were probably consumed by alcoholic fermentation to form ethanol while stored

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at the winery. This is confirmed by the initial ethanol content of 3.914 g/l. After 14 days and a month, the ethanol value dropped to 2.390 g/l and 1.890 g/l, due to acetic fermentation to form acetic acid, the concentration of which increased from 0.649 g/l to 2.392 g/l and 3.733 g/l after 2 weeks and a month, respectively. These found concentrations justify the choice of ethanol and acetic acid as the dominant contaminants, since their theoretical oxygen consumption approximately corresponds to the measured COD values (with typical deviations of less than 10 %). The volatility of individual contaminants affects their respective concentrations in the distillate from evaporation. While ethanol evaporates very easily, the concentration of acetic acid will be significantly lower in the distillate and the sugars will remain exclusively in the evaporation residue (concentrate). In the stripping step, it is then possible to effectively separate the binary ethanol-water mixture, but the possible presence of dissociating acetic acid negatively affects the quality of both products (ethanol and stripped water). The results clearly show that the storage time can have a decisive effect on the performance of the technology based on evaporation and stripping. At the same time, it is possible to optimize the storage time to achieve a certain technological goal.

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Early-warning System Development for Drinking Water Supply Using Statistical Approaches

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Drinking water quality can be represented by a variety of physical, chemical and biological parameters. Their monitoring is an essential part of the drinking water supply chain. To monitor them, drinking water suppliers are using time-consuming and costly methods. To supplement these methods, on-line monitoring of selected parameters helps to ensure higher quality control. However, these on-line early-warning monitoring systems have some disadvantages such as high price, lack of data analysis, need for reagents together with toxic waste generation and often just a single parameter monitoring. Nowadays, there are some reagent-free real-time monitoring systems already in use among a small number of drinking water suppliers and their use is rather considered as experimental.

Development of early-warning system for drinking water supply based on statistical modelling and utilization of sensors already available can provide a cheaper, more suitable alternative and fill the gap in the market. This presentation deals with our preliminary study, water quality data in Czech Republic and pilot testing of selected optical sensor. This lab-scale pilot considers the need for use of reagent-free methods and thus do not produce unnecessarily toxic waste, therefore provides a sustainable alternative to commercially available monitoring systems. Future work is needed to verify and up-scale this approach with an appropriate validation methodology considering potential risks.

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Study of the elemental composition of fly ash and bottom ash formed after the combustion of alternative lignocellulosic fuels

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Biomass energy is attracting more and more attention worldwide because it is a potentially CO_2 neutral and renewable energy source. Direct combustion is the conventional and most common way in which biomass is used to generate energy. The ash produced during the burning of lignocellulosic fuels consists of two main parts: fly ash and bottom ash. Fly ash is the lightest-weight component. It rises with the flue gases and is captured by a boiler or incinerator's air contaminant control equipment. Bottom ash is the material that falls to the bottom of the burner unit. Depending on the technology, bottom ash can be of ash consistency or often is a semi-solid slag material. The chemical characteristics of ash remaining after biomass burning depend on the types and quality of the fuels burned and the operating conditions and technology of the biomass facility. Although burning of lignocellulosic fuels produces ash that is "cleaner" than coal-derived ash or municipal solid waste incinerator ash, the characteristics of this ash can be a concern for human health or the environment.

In this study elemental composition of fly and bottom ash produced during burning of sunflower, corn biomass and spruce wood under different conditions was investigated. Fly ash was captured on filters and together with the bottom ash they were mineralized in a microwave oven using nitric acid and hydrogen peroxide. Subsequently, the content of Cd, Tl, Sb, As, Pb, Cr, Co, Cu, Mn, Ni, V, Al, B, Ca, Fe, K, Mg, Na, P and Zn was determined in all samples with the use of ICP-MS and ICP-OES techniques. Based on the results, the possible use of bottom ash produced during burning of individual types of biomasses as fertilizer was considered, and the possible risk of environmental pollution by metals in the emerging fly ash was assessed.

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Thermophilic Gram-positive bacteria of the genus Aneurinibacillus: Unique producers of various PHA copolymers

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Polyhydroxyalkanoates (PHAs) are biodegradable, biocompatible, and non-toxic biopolymers produced primarily by microorganisms. They share similar properties with commonly used plastic materials (which are mostly derived from petrochemicals) and could replace them in multiple applications. The most produced PHA is poly(3-hydroxybutyrate), but due to its high crystallinity, it is a rather stiff and brittle material which limits its range of applications. However, when various monomers are incorporated into the PHA chain, the crystal structure of the biopolymer is partially disrupted, and the mechanical properties of the bioplastic are improved. Therefore, it is crucial to search for suitable PHA producers able to utilize various substrates and produce different PHA biopolymers.

Although the PHAs are a very promising group of polymers, these materials are currently unable to economically compete with conventional plastics. The competitiveness of PHA can be increased using extremophile producers, such as thermophilic bacteria. Due to their optimal growth temperature, the risk of contamination by other microorganisms is notably reduced. This can result in a reduction of expenses related to maintaining sterile environments.

New thermophilic PHA-producing bacteria were found using an original isolation procedure by Dr. I. Pernicová et. al. Based on the 16S RNA sequencing, these thermophiles were assigned to the genus Aneurinibacillus. The ability of aneurinibacilli to synthesize poly(3-hydroxybutyrate-co-4-hydroxybutyrate) was previously demonstrated. This study aimed to further test the PHA production diversity of these bacteria. Other PHA monomers were synthesized using lactones (γ-valerolactone, γ-hexalactone, and δ-valerolactone) and glycerol (4+4 g/L). Aneurinibacillus strains have been shown to have an unusual ability to incorporate several PHA monomers into the structure of the PHA. Among the compounds produced are 4-hydroxyvalerate (69.3 mol.% of total PHA content), 4-hydroxyhexanoate (31.9 mol.%), and 5-hydroxyvalerate (47.1 mol.%). Furthermore, it was proved that the produced copolymers are less crystalline compared to poly(3-hydroxybutyrate) and can thus exhibit more suitable mechanical properties for various applications. Thermophilic bacteria of the genus Aneurinibacillus are considered promising producers of interesting PHA copolymers and their potential will continue to be investigated.

Thermophilic Gram-positive bacteria of the genus Aneurinibacillus: Unique producers of various PHA copolymers

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Metabolic characterization of carotenogenic yeasts cultivated on waste products of food industry

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Main goal of this work were cultivations of carotenogenic yeasts with the aim of enhanced biomass, lipidic substances (such as carotenoids, ergosterol and coenzyme Q), and a lipid production.Selected yeast strains were Sporidiobolus pararoseus, Sporidiobolus metaroseus, Cystofilobasidium macerans, Rhodotorula glutinis, Rhodotorula mucilaginosa and Rhodosporidium toruloides.

Main idea was to implement circular economy approach using waste products (such as waste frying oil, spent coffee grounds, and waste coffee oil) as sources of carbon in the media and to find the optimal composition of the production media and to maximize the production of selected metabolites. The second phase of experiments consisted of cultivation on waste coffee hydrolysate and waste oil and subsequent optimalization of phosphorus and magnesium concentration in the media.

Overall results show that of the tested strains, the highest production capabilities on waste materials, were achieved by the Sporidiobolus pararoseus strain. All cultivations that took place in media with coffee hydrolysate and waste oil show better production of metabolites and biomass than yeasts in control media.

Acknowledgement

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Effect of selenium and cobalt ions on algal and cyanobacterial biomass and metabolite production

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The use of microalgae and cyanobacteria in biotechnology is increasing in popularity nowadays. Microorganisms are capable of producing various metabolites, among which we can include carotenoids and lipids. Many of these metabolites have antioxidant properties or properties that positively influence biological processes. These desirable properties make further use in the food or pharmaceutical industry possible.

The aim of the current experiments is the optimization of cultivation conditions and the application of suitable stress factors to produce more biomass and enhance the production of selected metabolites. Cultivations were conducted on algal strains Chlorella minutissima and Chlorella sorokiniana and cyanobacterial strain Arthrospira maxima in a basic medium with the addition of increasing concentrations of Se6+ and Co2+. The positive effect of the addition of Se6+ was most noticeable in Arthrospira maxima and Chlorella sorokiniana.

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Application of bacterial cellulose in biomedicine

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Bacterial cellulose (BC) is one of the most interesting polysaccharides which is produced by microorganisms. Compared to plant cellulose, BC is synthesized without residues of other molecules such as lignin, hemicellulose, and pectin. The purity of the synthesized BC gives it an indisputable advantage over plant-based cellulose, which requires complex isolation and purification.

BC is structurally composed of a dense and organized 3D network of fibrils that form porous layers. This biopolymer is characterized by high crystallinity, thermal stability and better mechanical properties compared to plant cellulose. BC can absorb a large amount of water, is non-toxic, biocompatible, and hypoallergenic. Thanks to its high porosity, BC is able to carry molecules such as functional substances (antimicrobial, antioxidant, anti-inflammatory, etc.) or beneficial microorganisms (like probiotics or postbiotics) and then deliver them to a specific target, e.g. food packaging or wound healing.

BC has enormous potential in a wide range of application. Currently, much attention is focused on using BC in the biomedical field. The versatility of this material demonstrates a wide range of individual possible applications, such as dressing materials and wound coverings, vascular grafts, scaffolds for tissue engineering or artificial blood vessels.

Non-modified BC has unique physical and mechanical properties. However, to make full use of the potential of BC, it is necessary to modify BC by various methods. By modification, the chemical structure, porosity, crystallinity, or fiber density are changed. With adequately designed modification, it is possible to significantly improve and adjust the resulting properties for a specific application.

This work deals with a comparison between non-modified BC membranes and modified BC membranes by a crosslinker. The research was focused on the point of morphology, water content, swelling profile, viscoelastic behaviour and adsorption capacity of BC. It was proved that BC could adsorb methyl orange or other anionic/cationic dyes. Composites intended for the targeted distribution of drugs can be prepared by adding antibiotics or other substances to the BC structures. However, the adsorption capacity of BC depends on the porosity and functional groups present on its surface. With a correctly chosen modification we can prepare a composite that will meet the specified requirements of particular applications.

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The influence of clarification methods on the final quality of grapevine wines

Alžběta Suská[1,2], Eva Vítová[2]

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Wine clarity is considered one of the basic parameters of quality wine. For this reason, the musts are clarified before fermentation.

The content of lees particles in must is determined by many factors, as e.g. vintage, maturity, variety, health/damage of the grapes; the subsequent technological processes used are also important. Clarification is a necessary technological step, especially for white and rosé musts. This step results in cleaner and better quality wines by reducing the content of harmful microorganisms, pesticide residues, heavy metals and mineral impurities such as dust or plant residues. However, on the other hand, an excessive clarification may have negative effects, mainly the reduction of volatile compounds content and consequently modification of sensory quality of wines. There are several clarification methods used in practice: sedimentation, centrifugation, filtration, ultrafiltration or flotation. Fining agents, e.g. bentonite, can be applied to promote agglomeration and settling of lees.

In this study, the influence of various clarification techniques (sedimentation, filtration and fining) on the course of alcoholic fermentation, chemical composition and sensory properties of produced model wine samples was investigated. Non-clarified must was used as control. Two white grape varieties, Riesling (Ryzlink rýnský) and Pinot Gris (Rulandské šedé), were selected and used to produce wine samples; the whole production process took place in a winery under standard conditions [4]. Finished wine samples were subjected to analyses.

The sensory evaluation was carried out by panel of six professional assessors using the International Union of Oenologists‘ 100-point scale, and aroma profiles of wines were compiled. Using Alpha FT-IR spectrometer and Miura One analyser, the basic chemical parameters – density, alcohol, glycerol, titratable acids, pH, reducing sugar, glucose and fructose, tartaric, malic, acetic and lactic acids content were assessed; further total phenolic content (Folin-Ciocalteu assay), total flavanol content (DMAC spectrophotometric assay), antioxidant activity (FRAP and DPPH assays) were evaluated.

From the results obtained we can conclude, that grape variety and degree of maturity had the greatest influence on the quality of wines. Riesling variety was sensorially better evaluated than Pinot Gris - floral, citrus and herbal notes predominated in Riesling, while floral, herbal and fruit notes with slight defective tones in Pinot Gris variety. The clarification process clearly has a positive effect on quality, as the control sample was sensorially the worst; sedimentation for 24 hours (Riesling) or fining by bentonite for 12 hours (Pinot Gris) can be recommend for practical use.

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Commercial application of microalgae and cyanobacteria extracts

Paulína Strečanská, Renata Uhlířová, Ivana Márová

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Microalgae and cyanobacteria are autotrophic organisms interesting due to the production of a wide range of active substances of interest such as carotenoids, chlorophylls, proteins, and phenolic compounds. The production of these substances predisposes them to use in the cosmetics and food industry. This work aimed to investigate this application potential from the point of view of determining the cytotoxicity of extracts from the microalgae and cyanobacteria [1,2]. Cell lines of immortalized human keratinocytes HaCaT and colorectal adenocarcinoma cells CaCo-2 served as a model of the skin and intestinal barrier.

Aqueous and ethanol extracts were prepared from cultivated and commercial biomass of the genus Chlorella and Spirulina, which were subsequently characterized in terms of the content of the above-mentioned active substances. The highest amount of Chlorophyll b and carotenoids were extracted into 96% ethanol. On the other hand, aqueous extracts showed the highest extraction yield and also antioxidant activity.

Aqueous extracts of cultured microalgae and cyanobacteria were therefore selected to determine cytotoxicity using the MTT test. LC50 on skin cells was over 30 vol. % for both extracts from microbial biomass, on intestinal cells it was determined even over 45 vol. %. The tested extracts are therefore considered to be suitable for use as additives eighter in the cosmetic and food industries.

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Impact of cold atmospheric-pressure plasma treatment on the yeast Candida glabrata

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Cold atmospheric pressure plasma (CAPP) technology has achieved a great deal of attention in recent years, due to its positive attributes, including high efficiency against a wide range of microorganisms, ease of operation, economic simplicity and also environmental friendliness. Various effects and also some mechanisms of inactivation of bacteria and tumor cells have been explained over the last decade but the effects and mechanisms of fungi inactivation have not yet been sufficiently investigated. The aim of this work is to verify the effects of chosen low-temperature discharges on the model yeast example C. glabrata, in order to establish basic plasma set-up for further studies and experiments in vivo and to expand a global knowledge about the antifungal effects of CAPP. This study focuses on the effects of CAPP on C. glabrata as a representative of non-albicans species with the intention of its inactivation in order to help the problematic sterilization of small medical devices and subsequently find a new treatment method for superficial infections caused by Candida.

In this study, 4 different discharges, namely: microwave discharges (unipolar and surface wave) in the form of plasma jets, transient spark and corona discharge in the form of corona pen were tested. All discharges were tested by direct application onto a 24-hour inoculum of C. glabrata inoculated on agar plates. The results were evaluated based on the size and stability of the inhibition zones formed in the post treatment cultivation. From the individual measurements optimal conditions for testing the inhibitory effects of low temperature discharges on the selected yeast were determined. The microwave discharges (unipolar and surface wave) were chosen to be the most effective in the inhibition of C. glabrata. The measurements were therefore pursued with these discharges under selected conditions corresponding to chosen application of sterilization of surface infections in living organisms. The unipolar microwave discharge was chosen to be the most effective discharge for the potential treatment of superficial candidiasis.

The results of this work prove significant inhibitory effects of CAPP on the yeast C. glabrata, within the limits of in vitro cultivation and the so-called flat biology. The overall inhibitory effects are directly proportional to the irradiation time, the magnitude of applied power and also the area covered by the discharge. In terms of the initial cell concentration an indirect dependency can be observed, but it can also be stated that this factor is less significant compared to the other examined factors.

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Tématický okruh materiálové vědy

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Synthesis of thiophene based derivatives with bio-inspired side chains for use in bioelectronics

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In recent decades, interest in the field of organic electronics has grown enormously, not only at the level of basic and applied research, but also in the commercial sphere. Devices developed on the basis of organic transistors laid the foundation for organic bioelectronics.

The essential component of organic bioelectronic devices is mainly polymer with a conjugated π-system. Currently used polymeric materials often carry modified thiophene motifs. Several such polymers have been developed, but they often show some limitations, including low sensitivity, stability, or biocompatibility. The synthesis of new suitably functionalized conductive and semiconductive polymers, i.e. their monomer building units, is one of the ways to minimize the limitations.

This work focuses on the synthesis of thiophene derivatives with new bio-inspired side. Their side chains carry one of four amino acids: L-alanine, L-proline, L-lysine or L-arginine. Amino acids are linked to the thiophene nucleus by glycol linkers of various lengths. The basic synthetic approach to the preparation of monomers was esterification under Steglich conditions.

An oligoglycol linker was chosen for the study due to several studies proving that the polyglycol side chains of polythiophenes improve their electrochemical properties. However, beyond a certain number of glycol units, the material becomes too hydrophilic and loses its internal order upon contact with the electrolyte, which is undesirable. To study this dependence, derivatives with different lengths of the oligoglycol linker were synthesized.

The design of the target materials was chosen so that the synthesized monomers could be polymerized under oxi-DArP (catalytic oxidative direct arylation polymerization) conditions. For some monomers, homopolymerization under these conditions has been investigated. The great advantage of the chosen method was the possibility of avoiding metalation and halogenation, which are often accompanied by reactions with flammable, toxic and dangerous reagents, which are also sensitive to the presence of atmospheric moisture/oxygen.

Synthesis of thiophene based derivatives with bio-inspired side chains for use in bioelectronics

Katsiaryna Arkhiptsava, Jan Richtár, Jozef Krajčovič

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In recent decades, interest in the field of organic electronics has grown enormously, not only at the level of basic and applied research, but also in the commercial sphere. Devices developed on the basis of organic transistors laid the foundation for organic bioelectronics.

The essential component of organic bioelectronic devices is mainly polymer with a conjugated π-system. Currently used polymeric materials often carry modified thiophene motifs. Several such polymers have been developed, but they often show some limitations, including low sensitivity, stability, or biocompatibility. The synthesis of new suitably functionalized conductive and semiconductive polymers, i.e. their monomer building units, is one of the ways to minimize the limitations.

This work focuses on the synthesis of thiophene derivatives with new bio-inspired side. Their side chains carry one of four amino acids: L-alanine, L-proline, L-lysine or L-arginine. Amino acids are linked to the thiophene nucleus by glycol linkers of various lengths. The basic synthetic approach to the preparation of monomers was esterification under Steglich conditions.

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Gold Nanostructures for Surface-Enhanced Raman Scattering

Markéta Benešová[1,2], Zdeněk Pilát[2], Silvie Bernátová[2], Ota Samek[2]

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Raman spectroscopy is a non-destructive analytical technique based on Raman scattering, which is an inelastic scattering of electromagnetic (EM) radiation during the interaction with electrons in chemical bonds. Raman-active molecular bonds are typical by their high polarizability and are associated with specific Raman signals. Therefore, most molecules have their typical Raman spectra, by which their presence in the sample can be identified. However, Raman spectroscopy is relatively insensitive, low concentrations of molecules often give a very weak response.

This drawback can be overcome by a technique known as surface-enhanced Raman spectroscopy (SERS), using noble metal (Au, Ag) nanostructures to amplify Raman spectroscopic signals by localized plasmon resonance, which is a coherent oscillation of electrons that arises from the interaction of metal nanostructures with EM radiation. The enhancement of Raman scattering takes place when the analyte is adsorbed on the surface of the nanostructures, in areas with intense EM field oscillations, so-called hot spots. Raman signal amplification of several orders of magnitude can be achieved, commonly 103, but in certain cases up to 1011-1014.

The goal of our work was to use different SERS-based techniques to analyze microorganisms. The analyses were performed both directly, by using SERS to amplify signals of bacterial metabolites, and indirectly, with so-called Raman tags (or SERS-tags). SERS-tags are gold nanoparticles (AuNPs) that have their surface modified with antibodies, which bind to a specific bacterial strain based on antibody-antigen affinity, and Raman reporter, a molecule which provides a specific and strong Raman signal amplified by SERS on the AuNPs. When the signal of Raman reporter is observed in a sample, it indicates that the selected bacterial strain is present.

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Channel Length Dictates the Output Performance of MAPbBr3 Planar-Type Photodetectors

Stevan Gavranovic[1], Jan Pospisil[1], Oldrich Zmeskal[1], Vitezslav Novak[2], Petr Vanysek[2], Klara Castkova[3], Jaroslav Cihlar[3] and Martin Weiter[1]

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It the time of global energy crisis, societies are forced to seek for solutions that lead to self-dependent energy system. The European Union’s regulations, especially Renewable Energy Directive (2009/28/EC) and REPowerEU plan, prove that renewables play tremendous roll in future energy strategies [1]. Solar power is the really spectacular achiever among renewables. As International Renewable Energy Agency shown, global net installed photovoltaic capacity overtook that of wind energy at the end of 2021. Over 157 TWh, or 16.7 % of global photovoltaic electricity was generated across the EU in 2021 [2]. Heart of most commercially used solar cells is pure silicon. However, silicon is not the only material capable of efficient light-to-current conversion. In the recent years, metal halide perovskites have become a rising star of optoelectronics with potential to enhance or even replace silicon in many practical applications (solar cells, photodetectors). These inexpensive and abundant materials have very intriguing properties (tunable bandgaps, large optical absorption coefficient, high electron and hole mobility, etc.), suitable for various applications: solar cells, photodetectors, LEDs [3]. In less than 13 years of active study of photoactive perovskite layers, the efficiency of solar cell grew from 3.8 % (2009) to remarkable 25.7 % (2021). In tandem perovskite-silicon solar cells they can achieve efficiencies around 30 % [4]. The EU, including others, recognized the great potential these materials have and financed many projects dealing with halide perovskites. The biggest among them, Perovskite Thin-film Photovoltaics (PERTPV) with funds of € 4 996 041 [5].

In our latest work [6], we focused our attention to methylammonium lead bromide (MAPbBr3), a member of the APbX3 perovskite family (A is monovalent cation such as Cs+, CH3NH3+ or HC(NH2)2+, X is halide such as Cl–, Br–, I–), that proved to be relatively stable and efficient in light-to-current transition in visible spectrum under ambient condition. More specifically, we studied the effect of channel length on the output performance and stability of planar-type photodetectors based on high-quality methylammonium lead bromide (MAPbBr3) single crystals. Such crystals, were synthesized via inexpensive, inverse temperature crystallization method and were further used for fabrication of planar Au/MAPbBr3/Au pho-

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todetectors with variable channel length (in the range between 125 μm and 25 μm). We used these devices to detect low intensity light in visible spectrum. Our findings point out that, the channel length has a profound impact on photocurrent densities and key detector parameters (responsivity R, external quantum efficiency EQE and specific detectivity D*).

In the studied five-fold electrode spacing, the photocurrent density increased over four-times, with decreasing active area of the devices. We attributed this effect is to intrinsic photocurrent amplification, happening in the planar photodetector architecture. The responsivity and external quantum efficiency also increased with decreasing active area of the device. On contrary, increasing channel length reduced intensity of the dark current and improved overall detectivity of the device.

Based on the calculated output parameters we determined the sample with lowest detection limit, i.e. Au/MaPbBr3/Au photodetector with channel length of 50 μm. This sample exhibited maximum output performance (R of 19.6 A W–1, EQE of 4 253 % and D* of 3.4×1012 cm Hz1/2W–1) at 200 nW cm–2, which is, to our best knowledge, the weakest light intensity detected using bulk MAPbBr3 single crystals. Moreover, the functional stability of this device showed minimal reduction of photodetection ability after 2 000 cycles, which makes it very promising for the next generation of optoelectronic devices.

Our results indicate that the MAPbBr3 single crystals have tremendous potential in the field of filter-free detection of visible light around 570 nm. In addition, we proved that the sample with channel length of 50 μm shows the best output performances of all prepared photodetectors. All gained knowledge could potentially accelerate halide perovskite's path to the global market.

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Electrochemical Corrosion of Low Carbon Steel in the Presence of Humic Acid

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Humic acids are a heterogeneous mixture of organic compounds that are naturally found in water and soil. In recent years, there has been a growing interest in the application of green fertilizers containing humic acids in agricultural activities. Humic acid was isolated from South Moravian lignite. Corrosion test was performed on a low-carbon steel using a potentiodynamic polarization test in 0.1 M NaCl. Results suggest that corrosion was initially promoted due to the formation of complex compounds of humic acids with released iron ions. After a long time, a positive effect of humic acid was observed as the corrosion resistance of low-carbon steel increased due to adsorption of humic acid.

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Hydrothermal Synthesis and Characterization of Calcium Phosphate-Based Coatings on Az31 Magnesium Alloy

Lenka Horáková, Leoš Doskočil, Jaromír Wasserbauer and Martin Buchtík

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The aim of this study is to assess the influence of process parameters during the hydrothermal synthesis of CaP coatings on their properties. The monitored parameters were deposition time, pH of the reaction mixture, and concentration of precursors in the reaction mixture. For the deposited CaP coatings on AZ31 magnesium alloy, the surface morphology and the number of structural defects were evaluated using scanning electron microscopy (SEM). Electrochemical corrosion properties were evaluated using polarization techniques in Hank's solution. The measurements and analyses showed that the best results were obtained for the sample prepared in a reaction mixture at 120 °C, pH 5 for a deposition time of 120 min, when the concentration of precursors in the reaction mixture was 0.30 M Ca(NO3)2·4H2O and 0.28 M NH4H2PO4. This sample reach the corrosion potential Ecorr 1470 mV and the corrosion current density icorr was 0.158 μA·cm 2.

Based on electrochemical impedance spectroscopy (EIS) deposited coating significantly increased the corrosion resistance of the substrate in the short term (24-48 h) as the polarization resistance increased. Long-term corrosion tests showed that after 48 h the corrosion medium partially passed to the Mg substrate when the polarization resistance sharply decreased.

The deposited CaP coating consisted of 70.62 at.% of oxygen, 15.44 at.% of calcium, 13.72 at.% of phosphorus, and 0.21 at.% of magnesium. Based on this data and data from X-ray Diffraction Spectroscopy (XRD) it was proved that this coating was composed of DCPD (dibasic calcium phosphate dihydrate) with a small amount of octacalcium phosphate (OCP) .

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Hot Air Cooling by the Silicon Carbide Shell and Tube Heat Exchanger with Baffles

Petr Horvát[1], Josef Kalivoda[2], Ondřej Krištof[3], Tomáš Svěrák[2], Jaroslav Vlasák[2]

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The chemical engineering processes of cooling gasses by the pilot plant shell and tube heat exchangers with tubes made of innovative material is the major topic of this work. The aim of the work is to verify the theoretical convenience of silicon carbide as a better heat transfer surface material compared with borosilicate glass, traditionally used well chemically resistant material characterized by two orders of magnitude worse thermal conductivity. Subsequent applications in processes of removal of gaseous air contaminants via liquid absorber is the motivation. Experimental data for both materials were compared as well as results from the theoretical computational model using the j factor, the correction factors for the baffles, and the correction for air humidity condensation (according to the Perry's chemical engineers' handbook).

Heat transfer on two exchangers with glass or carbide tubes and eight plastic baffles was examined under constant conditions by cooling the air by 50% propylene glycol in tubes with flow about 3 kg/s. Coolant flowed through the exchanger three times, the speed about 1,8 m/s was reached in 60 tubes of an inner diameter of 11 mm. So only laminar flow rates were observed (Reynolds number about 1100). The inlet coolant temperature was chosen to be just above 0 °C, about -7 °C and about -15 °C. Air flowed in shell of inner diameter 0,2 m. The air flow could be regulated by frequency changer, 150–300 kg/h were used for experiments with a step of 25 kg/h. This corresponds to the off-layer speed up to 3 m/s, when the Reynolds number is about 3000. The inlet air temperature was chosen to be about 15 °C, 35 °C, 55 °C and about 75 °C. The humidity of air could be increased by water stream influx with intensity 1,5 kg/h or 2,5 kg/h. Both heat transfer media flowed in a recycling loop.

Outlet temperature of streams and outlet air humidity were measured as well as air pressure drop in the exchanger, flow rate of both streams, input temperature of streams and pressure, temperature and humidity in the laboratory. So, then the experimental value of the heat transfer coefficient could be calculated from the air flow, heat capacity of air, temperature change of air, heat losses, mean temperature difference between heat transfer media and heat transfer surface.

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Heat losses to the surroundings from exchangers were estimated based on calculations from dimensionless criteria. Due to these losses, the temperature profile in the exchanger was changed significantly, so that the mean temperature difference did not longer correspond to the commonly used logarithmic computational relationship (LMTD), so LMTD value needs to be corrected.

For glass, the experimental heat transfer coefficient was about 25 % higher at maximum flow than the theoretical model indicates. In the case of silicon carbide, the experimental value is about 44 % higher than the theoretical. But, in the case of the lowest examined air flow, for carbide, the experimental data are only 8 % higher than the theoretical, and, for glass, the experimental data are 1 % lower than the theoretical. It was also confirmed that with increasing amounts of condensing humidity in the exchanger, the heat transfer coefficient of the dry air decreases by up to 4 % during the performed experiments (the outlet air temperature increases slightly). At lower temperatures and lower flow rates, the values of the heat transfer coefficient are affected by heat losses, so the experiments using thermal insulation were done and are being evaluated.

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Synthesis of 1,2-diketone Precursors of Photosensitisers for Artificial Photosynthesis

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The continuously rising overall energy demand brought humankind to a point where we face substantial problems. As threats like the global energy crisis caused by the deficiency and depletion of fossil fuels or the fallout of greenhouse gas emissions on Earth‘s climate become strongly evident, a significant challenge lies in the hands of the science community. Artificial photosynthesis is a promising solution. By mimicking natural photosynthesis, these energetically unfavourable processes provide light energy storage into the chemical bonds of molecules of so-called solar fuels, economically valuable substances like molecular hydrogen, methane, or methanol.

The artificial photosynthesis‘s bottleneck is photosensitisers, the compounds playing the inherent role of providing initial solar irradiation capture and consequent electron transfer through the system to a photochemically unreactive substrate.

The natural omnipresent yellow pigment riboflavin, generally known as vitamin B2, has been successfully applied as the photosensitiser in numerous light-driven reactions, including photosensitised oxidations in organic synthesis, environmentally significant photochemical degradations of water pollutants [1], and within the medical sciences for photodynamic therapy in cancer treatment [2]. Hence, the photosensitising properties issue from the core of the molecular structure of riboflavin, isoalloxazine.

Our research deals with its isomer, alloxazine and its derivatives; our research group has recently studied the synthesizability of [3-4]. Consequent optical and electrochemical properties evaluation uncovered a possible use as a photosensitiser for hydrogen and oxygen evolution, advantaging in low toxicity and potential biocompatibility.

We are currently preparing significant precursors for synthesising advanced visible and near-infrared-absorbing flavins with the mentioned properties. Designing of the molecules is based on quantum-mechanical modelling for possible photocatalytic activity prediction. The already tested synthetic approaches include benzoin condensation, Friedel-Crafts acylation, Sonogashira coupling or Weinreb amide use.

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The artificial photosynthesis‘s bottleneck is photosensitisers, the compounds playing the inherent role of providing initial solar irradiation capture and consequent electron transfer through the system to a photochemically unreactive substrate.

The natural omnipresent yellow pigment riboflavin, generally known as vitamin B2, has been successfully applied as the photosensitiser in numerous light-driven reactions, including photosensitised oxidations in organic synthesis, environmentally significant photochemical degradations of water pollutants [1], and within the medical sciences for photodynamic therapy in cancer treatment [2]. Hence, the photosensitising properties issue from the core of the molecular structure of riboflavin, isoalloxazine.

Our research deals with its isomer, alloxazine and its derivatives; our research group has recently studied the synthesizability of [3-4]. Consequent optical and electrochemical properties evaluation uncovered a possible use as a photosensitiser for hydrogen and oxygen evolution, advantaging in low toxicity and potential biocompatibility.

We are currently preparing significant precursors for synthesising advanced visible and near-infrared-absorbing flavins with the mentioned properties. Designing of the molecules is based on quantum-mechanical modelling for possible photocatalytic activity prediction. The already tested synthetic approaches include benzoin condensation, Friedel-Crafts acylation, Sonogashira coupling or Weinreb amide use.

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Rheological Characterization and Turbidity Measurement of Agarose Hydrogels Tuned by Surfactant Additions

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Agarose is a linear polysaccharide naturally occurring in algae which in aqueous environment under proper conditions can form a hydrogel structure. Agarose is a biocompatible material and thus is used in extracellular matrix modeling and tissue engineering. Moreover, agarose is also well-known for its application in electrophoresis and as a nutrient medium. Agarose chains are considered almost uncharged, however, a small amount of sulfate groups are presented in these molecules.

In this proposed work, an impact of interactions between these groups with various surfactant molecules on the rheological properties of agarose hydrogels was studied. For this purpose, cetyltrimethyl ammonium bromide (CTAB) as cationic surfactant, sodium dodecyl sulfate (SDS) as anionic surfactant and Tween 20 as nonionic surfactant was utilized. Whereas neither anionic nor nonionic surfactants additions showed any influence on the rheology properties of agarose hydrogels, CTAB reported a significant impact in broad range of surfactant concentration (0.1 to 200 mM) covering amounts over as well as below the critical micellar concentration. In these samples, the storage modulus (related to crosslinking density) was increased from 3660 ± 450 Pa up to 6670 ± 530 Pa for 20 mM CTAB. Moreover, significant change was observed also in the linear viscoelastic regions (related to stiffness of nodes) which were shifted to higher values of applied strains with any CTAB addition compared to a reference sample. This was attributed to ionic interactions between the negative groups on the agarose backbone with positively charged surfactant molecule which strengthen the hydrogel structure. This assumption was supported by the turbidity measurements, where the increase of CTAB concentration up to 2 mM led to higher turbidity due to forming of aggregates. Even higher CTAB concentrations further lowered the turbidity due to solubilisation of these parts with a help of increasing number of micelles.

It might be concluded, that even a small amount of negative sulfate groups presented on the agarose backbone can have a significant impact on the rheological behavior when reacting with positively charged surfactant molecules.

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Study of hybrid-doped BaTiO3 ceramics aging by impedance and modulus spectroscopy

Kryštof Koller, Petr Ptáček

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Ceramic PTCR thermistor, or so-called posistor, is used in electrical circuit as a semiconductive component. Its electrical resistance increases sharply in a specific temperature interval after reaching Curie temperature TC, at which the barium titanate undergoes phase transition from tetragonal ferroelectric phase to paraelectric cubic phase. Due to this property, the posistor is used in a wide range of electronic applications, including indestructible fuses serving as an overload protection in electric motors, self-regulating heating elements, or special applications such as compressor motor starters in refrigerators.

Disadvantage of PTCR BaTiO3 based ceramics is that one of its key parameters, resistance at room temperature R25, decreases with time. In literature, various of aging mechanisms are mentioned, most of which attribute this phenomenon to diffusion of oxygen vacancies.

Impedance spectroscopy is used to separate contributions of regions with different electrical properties, such as grain bulk and grain boundary, and modulus plots provide additional information that cannot be derived from the impedance plane.

In this work, impedance and modulus spectroscopy was measured in time steps to determinate, which region was the most responsible for aging process. Based on results of our measurement it can be said that only the grain boundary degrades with time. In addition, third contribution of unknown region was observed.

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Conducting Hydrogel Based on Novel Polymer Composite PEDOT:DBSA for Bioelectronic Applications

Romana Malečková[1], Šárka Tumová[1], Petr Smísitel[2], Lubomír Kubáč[3], Jiří Akrman[3], Michaela Pešková[4], Jan Víteček[4], Jaromír Hubálek[2], Martin Vala[1], Martin Weiter[1]

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Organic conducting materials in the form of thin films are commonly used in various bioelectronic devices for advanced diagnostics or cell stimulation, such as biosensors, neural probes, electrode arrays or ion pumps for selective drug delivery. This is possible thanks to the unique properties of these materials, especially their relatively good biocompatibility and mixed conductivity - the ability to conduct both ions and electrons. Because of this, such materials are able to transmit the signal between the biological environment and electronical device very well, in comparison to conventional inorganic materials. One of the main factors that influence this transmission are the physical and mechanical properties of the material in contact with the biological environment. Thin films are, however, very distinctive from biological tissue. Because of the minimum (or non) water content, thin films are very hard and rigid. When in contact with the biological tissue, such thin films often cause an inflammatory reaction or scarring at the interface between the device and the tissue, which can negatively affect signal transmission and thus reduce the efficiency of the entire device.

The answer to these problems could be conductive hydrogels based on organic conducting materials. Such hydrogels, due to the high water content possesses mechanical and physical properties very close to those of living tissue. Unlike commonly used hydrogels, such as gelatine or agarose, they are also electrically and ionically conductive and thus represent an ideal material for creating an interface between the biological environment and electronic device.

In this work, we prepared a conductive hydrogel for use in regenerative medicine based on a completely new polymer composite – PEDOT:DBSA. The rheological characterization revealed that the mechanical strength of the hydrogel as well as the gelation time can be easily tailored to the desired application by changing the amount of cross-linking agent. The LDH biocompatibility assay of xerogels sho-

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Melt processing of poly(3-hydroxybutyrate) with isocyanate, carbodiimide, alcohol and epoxy reagents

Veronika Melčová, Štěpán Krobot, Vojtěch Jašek, Radek Přikryl

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A serious problem of poly(3-hydroxybutyrate) is its low thermal stability and narrow processing window. Upon heating to temperatures between 170 and 200 °C, the typical processing temperatures, the random chain scission of PHB is firstly manifested by the change in molecular weight and viscosity. During the degradation, two sub-molecules are formed, one with unsaturated crotonate end group, and the other with a carboxylate end group, which can be exploited for further reactions.

A laboratory kneader was used to study the processing changes of poly(3-hydroxybutyrate) in the melt with and without the addition of selected reagents with different chemistry: isocyanates, carbodiimides, alcohols and epoxides; and functionalities: from two to polyfunctional. Prepared samples with varied amount of the additives were characterised by means of processing performance, molecular weight and thermal properties determination, and some profound changes were observed.

Generally, bifunctional additives showed a higher increase in torque values at the end of the processing compared to the reference for the higher tested dosage, as expected due to the higher probability of the additive finding two polymer ends. The highest value was measured for carbodiimide reagent Stabaxol® 1 LF, 45% higher than neat PHB. In addition, the relative torque during kneading of the sample with 10-fold overdose of Stabaxol surpassed the reference during the whole processing time. Hexamethylene diisocyanate, bis(2,6-diisopropyl-phenyl)carbodiimide and diglycidyl ether of bisphenol A in 10-fold molar overdose towards PHB chain also led to 13–16% higher weight average molecular weight compared to the reference.

Trifunctional additives were effective in increasing the absolute values of processing torque and compensating for the loss of molecular weight in all tested dosages. Quite surprisingly, they were the most effective in the smallest amounts tested, as manifested by a profound change in the slope of the relative processing torque. This is caused by the plasticizing effect of the reagents in higher dosages. Nevertheless, glycerol in 2-fold dosage exhibited more than two times higher torque after 5 minutes of kneading at 185 °C than the reference. Moreover, it reached the highest molecular weight measured as well – 44% more than the neat PHB.

The effect of polyfunctional additives on final processing torque and molecular weight increases with higher dosages with few discrepancies. The highest num-

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Overall, some of the studied compounds showed to be promising candidates for PHB chain extension as their addition really caused profound changes in PHB processing performance and the resulting properties of the material.

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Porphyrin spiro-Tröger‘s Bases: Molecules for Chiral Recognition and Photodynamic Therapy of Cancer

Tereza Navrátilová and Bohumil Dolenský

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At the beginning of the 21st century, spiro-Tröger’s base (spiroTB), i.e. the constitutional isomer of the well-known Tröger’s base (TB), was discovered. To date, only five spiroTB derivatives have been described. In 2012, we discovered that the formation of the nickel(II) complex of porphyrin TB is accompanied by the formation of spiroTB, which was the only known spiroTB molecule that contained a porphyrin core in its structure. Here we present preparation of a series of new porphyrin spiroTB derivatives with different meso-aryl substituents as nickel(II) complexes or as free base molecules.

Enantiomers of the prepared nickel(II) complexes were separated using a chiral HPLC. We found, that the enantiomers of spiroTB show better chiral resolution in comparison to the enantiomers of TB analogues. This suggests that spiroTB could perform better than traditional TB in chiral recognition applications. Moreover, we successfully resolved the enantiomers of spiroTB on a preparative scale and measured their ECD spectra for the first time.

Free base porphyrin spiroTB derivatives were successfully prepared for the first time. We found, that free base derivatives of spiroTB show intensive absorption bands at around 675 nm of the radiation spectra. This absorption band is located in the area of the so-called phototherapeutic window (650 850 nm), which makes these compounds attractive as possible photosensitizers for photodynamic therapy of cancer.

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Color-Tunable Solid-State Fluorescence of Crystalline Powders Formed from Push-Pull Substituted 2,5-Diphenyl-Stilbenes

Rastislav Smolka[1], Karel Pauk[2]; Stanislav Luňák Jr.[1], Aleš Růžička[3], Aneta Marková[1], Kateřina Teichmanová[2], Anna Mausová[2], Matouš Kratochvíl[1], Tomáš Mikysek[4], Martin Weiter[1], Aleš Imramovský[2], Martin Vala[1]

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Photoluminescent materials based on organic conjugated molecules have attracted much attention due to their applications in various fields such as biological probes, chemical sensing and optoelectronic systems. The strong solid-state fluorescence (SSF) of such materials with emphasis on single-crystal emission is of importance for light-emitting field-effect transistors, stimuli responsive materials, organic light-emitting diodes (OLEDs) and water-dispersible nanoparticles in biomedicine and live-cell microscopy. The efficiency of SSF depends on the combination of intermolecular and intramolecular processes that can cause either quenching or enhancement of photoluminescence quantum yield (PLQY). Therefore, to understand and effectively utilize the relationship between the optical properties of materials and their modified structure is very much desired. In this work, the optical properties of a series of new π-conjugated DPA DPS EWG (DPA – diphenylamino, DPS – 2,5-diphenyl-stilbene building blocks, EWG – electron withdrawing group) were investigated. By varying the strength of the EWG, the LUMO energy could be tuned, resulting in a change of the SSF maxima in the interval from 380 nm to 630 nm, covering a range of 250 nm. These results demonstrate the potential of such an approach for the development of multicomponent white-light-emitting materials.

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Influence of Pt Nanoparticles on Fulvic Acids

Matěj Šram[1], Renata Komendová[2]

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Nanoparticles abound with unique properties due to their large specific surface. These properties have earned them great popularity in most fields, ranging from medical, energy, electronics, and environmental applications to personal care products and food industry. The large-scale application of nanoparticles is accompanied by their abundant release into the environment during their lifecycle, including production, transport, storage, application, and final disposal. In addition, nanoparticles created as a by-product of human activity contribute to nanoparticle emissions. Pt nanoparticles are mostly used in medical and catalytic applications, but the main emission sources are automotive catalysts of which they are a by-product.

Environmental implications caused by nanoparticle pollution are not very well understood yet.

In this study we focus on how fulvic acids are influenced by nanoparticles. Fulvic acids are an essential part of the environment. They influence a wide spectrum of biogeochemical processes such as solubilization, energy and nutrient supply, surface water photochemistry, plant growth or biotransformation of xenobiotics.

It has been shown, that fulvic acids change their physical conformation due to temperature changes. After being exposed to heating and cooling cycle there is a slow structural relaxation.

In this study six fulvic acids with various concentrations of Pt nanoparticles were analyzed by measuring ultrasonic velocity and density to evaluate the adiabatic compressibility. Structural relaxation times were obtained from the measurements. Pt nanoparticles seem to interact mostly with the aliphatic chains of the fulvic acids. There was observed an increase of the structural relaxation time when the aromaticity of the fulvic acid was low.

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Nanoparticles abound with unique properties due to their large specific surface. These properties have earned them great popularity in most fields, ranging from medical, energy, electronics, and environmental applications to personal care products and food industry. The large-scale application of nanoparticles is accompanied by their abundant release into the environment during their lifecycle, including production, transport, storage, application, and final disposal. In addition, nanoparticles created as a by-product of human activity contribute to nanoparticle emissions. Pt nanoparticles are mostly used in medical and catalytic applications, but the main emission sources are automotive catalysts of which they are a by-product.

Environmental implications caused by nanoparticle pollution are not very well understood yet.

In this study we focus on how fulvic acids are influenced by nanoparticles. Fulvic acids are an essential part of the environment. They influence a wide spectrum of biogeochemical processes such as solubilization, energy and nutrient supply, surface water photochemistry, plant growth or biotransformation of xenobiotics.

It has been shown, that fulvic acids change their physical conformation due to temperature changes. After being exposed to heating and cooling cycle there is a slow structural relaxation.

In this study six fulvic acids with various concentrations of Pt nanoparticles were analyzed by measuring ultrasonic velocity and density to evaluate the adiabatic compressibility. Structural relaxation times were obtained from the measurements. Pt nanoparticles seem to interact mostly with the aliphatic chains of the fulvic acids. There was observed an increase of the structural relaxation time when the aromaticity of the fulvic acid was low.

Synthesis and Study of New Regioregular Polythiophenes with Adamantyl Side Chains for Organic Electronics

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Since their discovery in 1977 by Nobel prize laureate Alan Heeger and his team, the investigation on organic conjugated polymers is the subject of many studies around the globe. These unique materials attract big attention as they possess great optical, electrical, morphological, and mechanical properties. Moreover, these lightweight and easy-to-process materials can be utilized in different thin, large-scale, mass-produced, and flexible devices. They already have huge impact in the daily life in applications like organic transistors, organic light-emitting diodes, sensors, or photovoltaic devices and their character makes them serious competitors to the conventional inorganic materials. Nevertheless, there are still some drawbacks and challenges that needs to be deal with where probably the most important characteristic is the overall performance of these organic materials, which can be readily solved by molecular structure tailoring.

Polythiophenes are among the most studied conjugated polymers in the field of organic electronics, however the plain polymer backbone of unsubstituted thiophene units is semiflexible and forms strong aggregations which leads to insolubility. This massive processability issue is usually solved by the side chain substitutions that, besides positively impacting the formation of self-assembled structures thanks to the intra- and interchain interactions, can also enhance the overall optical, electrical, and electrochemical properties. By this way, the 3-alkylated polythiophenes gain great scientific interest, where mainly linear or branched alkyl derivatives are the subjects of the research.

This work focuses on the synthesis and study of optical and electrical properties of two novel regioregular poly(3-adamantylmethylthiophene) (PMAT) and poly(3-adamantylethylthiophene) (PEAT) polymers, characterized by a bulky adamantane side group. These thermally and chemically stable materials show good solubility in common organic solvents hence are convenient for upscaling, industrial processing, and production of stable and long-life devices. The molecular ordering was investigated by the GIWAXS technique, the experiments confirmed the presence of both crystalline and amorphous phases. While the charge carrier mobilities are comparable to the reference poly(3-hehylthiophene) (P3HT), on the other hand the absorption and emission measurements indicate less flexibility in rotation of the adamantyl-methyl/ethyl side groups both in solution and in thin-la-

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Key words

Side substituents, solution-processable polythiophenes, GIWAXS, charge-carrier mobilities.

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Relationship between the structure and ballistic resistance of RPC composites

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This work deals with „Relationship between the structure and ballistic resistance of RPC composites“ deals with cementitious composites based on RPC (Reactive powder concrete) with a focus on the final mechanical properties. In contrast with traditional quasi-static loading, this work deals with high-velocity dynamic loading with a focus on resistance to ballistic loading. In order to achieve increased resistance to dynamic stress, it is necessary to optimize the granulometry of the filler and the use of high-strength aggregate, significantly reducing the water content and the use of superplasticizers. The response of the cementitious composite to dynamic stress can be monitored by a ballistic test. The resistance to ballistic loading is monitored by depth of penetration (DoP - Depth of Penetration) after the impact of the projectile on the cementitious composite.

This work deals with the optimization of particle size distribution of fillers and the preparation of cementitious composites under reduced pressure (porosity reduction) using fiber reinforcement. These parameters are monitored by traditional mechanical tests for building materials and ballistic tests to monitor the response to high-velocity dynamic loading.

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Structural and Transport Properties of Hybrid Hydrogel Based on Sodium Alginate and Polyvinyl Alcohol

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Nowadays the interest in the study of hydrogel is constantly growing, as these gel systems find application in various sectors of human activity. Hydrogels are ionically, chemically and/or physically cross-linked polymers with a three-dimensional network structure, which is able to absorb and hold large amount of water or biological fluids to a thousand times of their own weights. This property makes them the ideal candidate for various applications, such as tissue engineering, wound healing, drug delivery systems, biosensors and bioelectronics, wastewater remediation, daily life product and so on.

This work is focused on the preparation and subsequent characterization of structural and transport properties of hydrogels with the double-network structure concerning their application potential. With regard to already existing research papers, hybrid hydrogels were prepared as a combination of synthetic polymer and natural polysaccharide, such as polyvinyl alcohol (PVA) and sodium alginate (ALG). In the preparation of this gel's hybrid network a freeze-thawing cycle technique for physical cross-linking of PVA was used. Also, calcium ions were used for ionic cross-linking of sodium alginate. Another part of this work is tailoring of the internal structure of hybrid hydrogels with lecithin as a model of the phospholipid bilayer, forming the cell membrane or occurring in tissue.

Physicochemical methods were used to characterize their viscoelastic, swelling and transport properties. Rheology measurements, specifically oscillation and amplitude tests, were used to study these viscoelastic properties. Morphology of the prepared hybrid hydrogels was confirmed by electron microscope scanning. Transport and release properties of gel systems were determined by diffusion experiments with the UV-VIS spectrometry detection, in which an organic dye (methylene blue) was used as a model probe.

The results present that all the measurement data indicate that sodium alginate, or lecithin affects the properties and structure of the hydrogel, which make it possible to alter the properties of hybrid gel systems according to the required applications.

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