studentská konference

CHEMIE JE ŽIVOT

25.–26. 11. 2021

SBORNÍK ABSTRAKTŮ

VYSOKÉ UČENÍ TECHNICKÉ V BRNĚ
FAKULTA CHEMICKÁ

Studentská odborná konference
CHEMIE JE ŽIVOT 2021
Sborník abstraktů

Editor: Ing. Petr Dzik, Ph.D.
Nakladatel: Vysoké učení technické v Brně, Fakulta chemická,
Purkyňova 464/118, 612 00 Brno

Vydání: první
Rok vydání: 2021
Náklad: elektronicky
ISBN 978-80-214-6002-7
Tato publikace neprošla redakční ani jazykovou úpravou

OBSAH

SEKCE STUDENTŮ STŘEDNÍCH ŠKOL

SEKCE STUDENTŮ BAKALÁŘSKÝCH A MAGISTERSKÝCH PROGRAMŮ

SEKCE STUDENTŮ DOKTORSKÝCH PROGRAMŮ

1) Life Science - Sekce organické, environmentální chemie a biochemie

SEKCE STUDENTŮ DOKTORSKÝCH PROGRAMŮ

2) Material Science - Sekce analytické, anorganické a materiálové chemie

SEKCE
STUDENTŮ
STŘEDNÍCH ŠKOL

Studium elektrochemického chování sekundárních struktur oligonukleotidů adsorbovaných na povrchu elektrody z pyrolytického grafitu

Ondřej Chytrý ☻

Střední průmyslová škola chemická Brno, Vranovská,
příspěvková organizace

Studýnka 59, Omice 66441
chytry.ondrej@seznam.cz

Nukleové kyseliny mohou vytvářet různé sekundární struktury. Kromě obecně známé dvoušroubovice mohou úseky deoxyribonukleové (DNA) nebo ribonukleové kyseliny (RNA) o vhodné nukleotidové sekvenci zaujmout tzv. alternativní struktury, např. křížové formy, triplexy nebo guaninové (G4) či cytosinové kvadruplexy (tzv. I-motivy). Jsou-li tyto struktury vytvářeny v určitých místech genomové DNA (např. v promotorových oblastech genů), mohou ovlivňovat důležité procesy (expresi příslušných genů). Díky moderním elektroanalytickým metodám, je možné nukleové kyseliny citlivě detekovat pomocí běžně používané rtuťové kapkové elektrody nebo nově využitím elektrody z pyrolytického grafitu (PGE)[1]. Ta díky svému širokému rozsahu využitelného potenciálu (−2,0 V až 1,6 V) umožňuje detekci jednotlivých bází nukleových kyselin i jejich produktů elektrochemické přeměny. Ověření možnosti jejího využití pro detekci sekundárních G4 struktur DNA pomocí PGE bylo podstatou této práce. Byl studován vliv podmínek (složení elektrolytu a velikost potenciálového okna) na detekci vybraných oligodeoxynukleotidů (ODN) pomocí cyklické voltametrie v prostředí 0,2 mol.l^{-1} acetátu sodného nebo amonného pufru pH 5,0. Pro následná měření byl zvolen 0,2 mol.l^{-1} amonno-acetátový pufr pH 5,0, ve kterém ODN poskytovaly nevyšší redoxní signál guaninu[2]. V tomto pufru byly dále zkoumány výšky všech dostupných redoxních signálů ODN adsorbovaných na PGE ve vztahu k jejich předpokládané sekundární formě, které v roztoku za vhodně zvolených podmínek tvoří. Výsledky této práce dokazují nemožnost rozlišení mezi jedno-vláknovou, dvou-vláknovou a G4 formou ODN využitím voltametrického měření na PGE. Důvodem může být nedostatečná stabilita sekundárních struktur po jejich adsorpci na povrchu elektrody nebo rozpad sekundární struktury vlivem vloženého potenciálu. Podrobnější studium bude součástí navazující práce.

Literatura

[1] Barek, J.; Opekar, F.; Štulík, K. *ELEKTROANALYTICKÁ CHEMIE*.

[2] Špaček, J.; Daňhel, A.; Hasoň, S.; Fojta, M. Label-Free Detection of Canonical DNA Bases, Uracil and 5-Methylcytosine in DNA Oligonucleotides Using Linear Sweep Voltammetry at a Pyrolytic Graphite Electrode. *Electrochem. commun.* **2017**, *82* (July), 34–38. https://doi.org/10.1016/j.elecom.2017. 07. 013.

Poděkování

Tímto bych chtěl velice poděkovat vedoucímu mé práce panu RNDr. Aleši Daňhelovi, Ph.D. z Biofyzikálního ústavu (BFÚ) Akademie věd České republiky z Oddělení biofyzikální chemie a molekulární onkologie především za jeho velkou ochotu, trpělivost a spoustu věnovaného času při práci, skvělou spolupráci i za ohromný přísun znalostí.

Fluorescenční spektroskopie ve výzkumu modelových systémů pro cílenou distribuci léčiv

Martina Ruttkayová

Střední průmyslová škola chemická Brno, Vranovská,
příspěvková organizace

Nálepkova 97, Brno – Jundrov 637 00
martina.ruttkayova@seznam.cz

Simona Patloková

Tato práce se snaží objasnit alespoň částečně základy výzkumu cílených nosičů léčiv, které je možno využít například při léčbě rakoviny. Jednou z metod léčení rakoviny je například chemoterapie. Tento typ léčby zasahuje celé tělo a dochází k celkovému oslabení organismu. Chemoterapie je pro tělo mnohdy větší zátěží než nemoc sama. Cílené nosiče nepůsobí na celé tělo, ale účinkují pouze v oblastech zasažených rakovinným bujením. Na vyvinutí léčby pomocí cílených nosičů léčiv pracují výzkumníci na celém světě, protože by měla eliminovat nežádoucí účinky chemoterapie na lidský organismus.

Zaměřily jsme se tedy na metodu fluorescenční sondy v oblasti vývoje cílených nosičů léčiv. Fluorescence je zde využita hlavně k charakterizaci modelů pro cílenou distribuci léčiv. Zkoumané modelové nosiče léčiv jsou založeny na elektrostatické interakci kladně nabitých agregátů tenzidu a opačně nabité hyaluronové kostry. Součástí této práce je seznámení se s výzkumem pomocí fluorescenční sondy. Dále jsou zde měřena fluorescenční spektra pyrenu ve vybraných modelových systémech. Cílem je práce zjistit různá chování tenzidu a vytvořených micel v určitých simulovaných prostředích.

Literatura

[1] Cílený transport léčiv [online]. Vysoká škola chemicko-technologická v Praze, 2017 [cit. 2020-01-10].

[2] ŠIMEČKOVÁ, Marie. Transport platinových cytostatik do buněk [online]. [cit. 2020-01-07]. Univerzita Palackého v Olomouci, přírodovědecká fakulta. Vedoucí práce Prof. R NDr. Viktor Brabec, DrSc.

Poděkování

V prvé řadě bychom chtěly poděkovat naší vedoucí práce Ing. Tereze Venerové, Ph.D., za její trpělivost a odborné vedení. Také bychom jí chtěly poděkovat za ochotu, podporu a umožnění práce v laboratoři fyzikální chemie při VUT v Brně.
Dále bychom chtěly poděkovat Mgr. Tereze Důbravové za konzultaci a rady k naší práci. Také děkujeme našim rodičům a přátelům za trpělivost a podporu během naší práce.

SEKCE STUDENTŮ BAKALÁŘSKÝCH A MAGISTERSKÝCH PROGRAMŮ

Má lignín antibakteriálne vlastnosti?

Martin Chovanec[1], Pavel Vostrejš[2], Adriana Kovalcik[3]

[1] Ústav chemie potravin a biotechnologií, Fakulta Chemická, VUT v Brně

Purkyňova 118, Brno, Česká republika
xcchovanecm@vutbr.cz

[2] Ústav chemie potravin a biotechnologií, Fakulta Chemická, VUT v Brně

Purkyňova 118, Brno, Česká republika

Ligníny sú aromatické biopolyméry s amorfnou štruktúrou zložené z fenylpropánových jednotiek s rôznymi funkčnými skupinami. Základná funkcia lignínu v rastlinách je ochranná a stužujúca funkcia cievneho systému. Antibakteriálna aktivita extraktov z rozličných lignocelulózových rastlín je všeobecne akceptovateľná [1]. Avšak ligníny sú heterogénne a po izolácii z rastlín majú fyzikálne a chemické vlastnosti odlišné od „natívneho lignínu“ prítomného v bunkových stenách rastlín. Jednoznačná štruktúra lignínu doposiaľ nebola popísaná.

V tejto práci bola skúmaná hypotéza, že sóda lignín izolovaný z hroznových výliskov by mohol mať antimikrobiálne vlastnosti [2]. Izolácia lignínu prebiehala pomocou tzv. sódového rozvlákňovania (soda pulping) [3], prebiehala dvoma spôsobmi a to za použitia laboratórnej aparatúry za atmosferického tlaku a pomocou hydrotermálneho autoklávu, vyrobeného pre túto prácu. Následne bola porovnaná efektivita týchto metód, pričom efektívnejšia bola izolácia lignínu v hydrotermálnom autokláve, s výťažnosťou 36,35 g lignínu na 100 g hroznových výliskov. Zároveň bola pomocou FTIR preukázaná vyššia čistota takto izolovanej vzorky. Lignín izolovaný oboma spôsobmi nemal antimikrobiálne vlastosti, čo bolo preukázané pomocou jamkovej difúznej metódy. Následnou modifikácou lignínu časticami striebra bola dosiahnutá antibakteriálna aktivita, avšak žiadna zo vzoriek nepôsobila proti kvasinkám. Antimikrobiálna aktivita bola testovaná na baktériách *Bacillus subtilis, Escherichia coli, Micrococcus luteus, Serratia marcescens* a kvasinkách *Saccharomyces cerevisiae* a *Candida glabrata*, pričom najvyššia aktibakteriálna aktivita bola zaznamenaná pri *Micrococcus luteus*.

V tejto práci bolo zistené, že lignín izolovaný z hroznových výliskov je možné modifikovať naviazaním častíc striebra a tým dosiahnuť jeho antibakteriálne vlastnosti voči gram-pozitívnym aj gram-negatívnym baktériám.

Literatúra

[1] A. Gregorova, Lignin: Antibacterial Properties, in: M. Mishra (Ed.), Encyclopedia of Biomedical Polymers and Polymeric Biomaterials, Taylor & Francis, CRC Press Inc2015, pp. 4328-4334.

[2] T.V. Lourençon, G.G. de Lima, C.S. Ribeiro, F.A. Hansel, G.M. Maciel, K. da Silva, S.M. Winnischofer, G.I. de Muniz, W.L. Magalhães, Antioxidant, antibacterial and antitumoural activities of kraft lignin from hardwood fractionated by acid precipitation, International Journal of Biological Macromolecules 166 (2021) 1535-1542.

[3] T.V. Lourençon, G.G. de Lima, C.S. Ribeiro, F.A. Hansel, G.M. Maciel, K. da Silva, S.M. Winnischofer, G.I. de Muniz, W.L. Magalhães, Antioxidant, antibacterial and antitumoural activities of kraft lignin from hardwood fractionated by acid precipitation, International Journal of Biological Macromolecules 166 (2021) 1535-1542.

Poďakovanie

Táto práca bola podporená interným grantom FCH VUT č. FCH-S-21-7440.

Konstrukce jednoduchého syntetického bakteriálního konsorcia s dělbou práce

Stanislav Juračka[1], Pavel Dvořák[1]

[1] Laboratoř bioinženýrství mikroorganismů, Ústav experimentální biologie (Oddělení mikrobiologie), Přírodovědecká fakulta, Masarykova univerzita,

474088@mail.muni.cz

Mikrobiální konsorcium je soužití dvou nebo více odlišných mikroorganismů, které spolu nějakým způsobem interagují. Téměř každý volně žijící mikroorganismus na planetě žije v nějakém druhu mikrobiální komunity. Díky této životní strategii se může člen konsorcia odprostit od náročného života samotáře a specializovat se na jeden daný úkol. Toto označujeme jako princip dělby práce. V posledních letech rapidně roste zájem o mikrobiální konsorcia v oblastech biotechnologií a syntetické biologie. Ve srovnaní s klasickým využitím pouze jednoho kmene dělba práce teoreticky zvyšuje výtěžek koncového produktu a odolnost buněk vůči stresu. [1]
Cílem prezentovaného projektu je vytvořit jednoduché mikrobiální konsorcium složené ze dvou rekombinantních kmenů biotechnologicky atraktivní bakterie *Pseudomonas putida*. Konsorcium bude využívat principu dělby práce. Je navržené tak, aby jako zdroj uhlíku bylo schopné zpracovat modelový polymerní substrát karboxymetyl celulózu (CMC), která simuluje odpadní rostlinou biomasu, a z ní generovalo cílový produkt s vyšší přidanou hodnotou. První kmen produkuje celulolytické enzymy, které jsou do prostředí vypuštěny indukovanou buněčnou lyzí. Enzymy následně začnou štěpit přítomný polymerní substrát. Druhý kmen roste na uvolněných monosacharidech a oligosacharidech a tvoří požadovaný produkt.

U mikrobiálních systémů s indukovanou buněčnou smrtí je často problém s bazální expresí smrtícího genu. Proto je v této diplomové práci vyzkoušen nový systém řídící expresi genu, takzvaný digitalizační modul. Modul zajišťuje, aby k expresi toxického genu docházelo jen a pouze v přítomnosti specifického induktoru. [2]

Zatím se nám podařilo metodami genetického inženýrství připravit základ pro plánované konsorcium – dva kmeny *P. putida* označené zeleným a červeným fluorescenčním proteinem. Do kmene s červeným fluoroforem byl vložen plasmid s digitalizačním modulem a lytickým genem a byla testována jeho funkce. Buněčné kultury jsou analyzovány spektrofotometricky v mikrotitračních destičkách a pomocí průtokové cytometrie.

Dalším krokem je dokončení přípravy rekombinantních kmenů a otestování jejich funkcí samostatně. Následně budou kmeny skombinovány v syntetickém konsorciu, jehož chování bude detailně analyzováno a srovnáno s kmenem, který bude všechny funkce konsorcia zajišťovat sám. Toto srovnání potvrdí či vyvrátí hypotézu o výhodnosti dělby práce u tohoto konsorcia.

Literatura

[1] Juračka S., Bakalářská práce, Vedoucí práce Dvořák P., Masarykova univerzita Přírodovědecká fakulta, Brno 2020, https://is.muni.cz/th/qfnvf/

[2] Calles B. a kol., *Molecular Systems Biology* 15 (2019) e8777.

Poděkování

Velké poděkování míří především vedoucímu diplomové práce Pavlu Dvořákovi a konzultantce Barboře Burýškové za trpělivost, zázemí a cenné rady, které autorovi poskytují, a Grantové agentuře Masarykovy univerzity (MUNI/C/1811/2020) a Grantové agentuře České republiky (19-06511Y), které na projekt poskytly finanční podporu.

Degradace biopolyesterů v simulovaných tělních tekutinách

Markéta Sobková[1], Adriana Kovalcik[2]

[1] Vysoké učení technické v Brně, Fakulta chemická, Ústav fyzikální a spotřební chemie

Purkyňova 118, 612 00 Brno, Česká republika
xcsobkovama@vutbr.cz

[2] Vysoké učení technické v Brně, Fakulta chemická, Ústav chemie potravin a biotechnologií

Purkyňova 118, 612 00 Brno, Česká republika

Povědomí o enviromentální zátěži petrochemickými polymerů vede k celosvětové snaze vyvíjet materiály s podobnými fyzikálně-chemickými vlastnostmi, které budou získávány z obnovitelných zdrojů a zároveň budou plně biologicky rozložitelné, a tudíž šetrné k životnímu prostředí. Budování trhu takovýchto biopolymerů vede k úvahám využívat tyto materiály nejen jako náhradu petrochemických polymerů pro průmyslové aplikace. Řada výzkumů jasně ukazuje, že jsou tyto materiály velmi vhodným kandidátem také pro aplikace biomedicínské.

Tradičně využívané materiály pro lékařské implantáty, jako jsou kovy, keramika nebo syntetické polymery, mohou v těle interagovat a projevovat se negativními imunologickými reakcemi. Často je nutnost provést druhou operaci pro jejich odstranění z těla pacienta. Biopolyestery, kterým se věnuje tato práce, jsou biokompatibilní, necytotoxické a podléhají biodegradaci, při níž dochází z rozkladu na tělu vlastní látky, které jsou v organismu dále metabolizovány nebo přirozeně vyloučeny z organismu ven, tudíž zde odpadá nutnost opětovně operativně zasahovat do těla pacienta pro odstranění podpůrného materiálu.

V této práci byla studována *in vitro* biodegradace dvanácti vzorků různých typů biopolyesterů – polykyseliny mléčné, polyhydroxyalkanoátů a poly(butylen adipát-*co*-tereftalátu). Tenké filmy, jež byly využity pro samotný experiment, byly připraveny rozpouštěním polymeru v chloroformu, vylitím do formy a následným odpařením rozpouštědla. Dle typu polyesteru a jeho stupně krystalinity se měnily vlastnosti připravených filmů, jejich vzhled byl v škále od transparentních do mléčně zakalených a mechanické vlastnosti se lišily především v elasticitě.

Studium degradace probíhalo ve dvou simulovaných tělních tekutinách, a to v syntetické žaludeční šťávě a ve fyziologickém roztoku pufrovaném fosfáty s lipázou při teplotě 37 °C po dobu 81 dní. Během degradace docházelo k viditelné změně morfologie filmů a studované vzorky získávaly vyšší stupeň křehkosti a nižší kompatibilitu.

Ze získaných výsledků lze potvrdit, že biodegradace u těchto biopolyesterů opravdu probíhá. Její průběh je ale závislý na mnoha proměnných faktorech, díky nímž je možno rychlost biodegradace korigovat a měnit, a tedy je možné předpokládat široké využití v mnohých biomedicínských aplikacích.

Poděkování

Prezentovaný výzkum byl finančně podpořen z interního projektu FCH VUT č. FCH-S-21-7483. Ráda bych poděkovala Ing. Michaele Jakešové (FCH VUT) za produkci a přípravu poly(-3-hydroxybutyrátu-co-3-hydroxybutyrátu), Ing. Michalu Kalinovi, PhD. (FCH VUT) za analýzu SEC-MALLS, Leoně Kubíkové (FCH VUT) za provedení DSC a Ing. Michalovi Machovskému (CPS UTB Zlín) za SEM mikroskopii.

Polymerní systémy s kolchicinem pro cílené dodávání léčiv

Markéta Štejdířová[1]

[1] Ústav počítačové a řídicí techniky, Fakulta chemicko--inženýrská, VŠCHT Praha

Technická 6, Praha 6, 166 28

Vývoj systémů pro dodávání léčiv založený na polymerních nanočásticích může řešit jednu z hlavních výzev při bojích s rakovinou, a to zlepšení biologické dostupnosti léčiva v těle. Hlavním cílem tedy je vytvoření takového systému, který podpoří cílení léčiva a umožní mu kontrolované uvolňování. Zároveň musíme myslet na velkou toxicitu cytostatických léčiv a na možnosti ochrany zdravých buněk.

Kopolymer kyseliny glykolové a kyseliny mléčné (poly(lactide-*co*--glycolide) - PLGA) patří k nejpoužívanějším biologicky odbouratelným polymerům pro jeho dobrou biologickou kompatibilitu a možnost kontrolovatelné degradace hydrolýzou. Další výhodou je možná úprava povrchu PLGA na požadované vlastnosti (např. zvýšení rozpustnosti). Uzavření kolchicinu do polymerního systému má potenciál z důvodu cytostatických účinků kolchicinu, ale zároveň pro snížení jeho vysoké toxicity.

Provoz, optimalizace a využití kapacitní deionizační jednotky

Jan Vespalec[1], Martina Švábová[1], Martina Repková[1]

[1] Vysoké Učení Technické v Brně, Fakulta chemická, Ústav chemie a technologie ochrany životního prostředí

Purkyňova 464/118, Královo Pole, 61200 Brno 12
Jan.Vespalec@vutbr.cz

V České republice je zásobováno 30 % obyvatel tvrdou vodou a 6 % obyvatel velmi tvrdou vodou [1], která může způsobovat problémy ve spotřebičích. Například v Brně máme přibližnou tvrdost 2,85 mmol/l [2]. K ničení spotřebičů dochází z důvodu tvorby nánosu v potrubí nebo vyloučením například uhličitanu vápenatého při varu vody [3].

Existuje více technologických řešení na změkčování pitné vody, mezi které nejčastěji řadíme membrány, iontoměniče [3] nebo námi studovanou kapacitní deionizaci. Kapacitní deionizace má v porovnání s membránovými procesy podstatně menší tlakové nároky, tím i nižší náklady na provoz. V porovnání s iontoměniči není potřeba používat žádné další provozní chemikálie.

Další praktické využití nalézá kapacitní deionizace při odsolování brakických vod, zejména při adsorpci alkalických kovů, kovů alkalických zemin a amoniaku. Z aniontů dochází nejčastěji k adsorpci halogenidů, dusičnanů, dusitanů a fosforečnanů. Rovněž se uplatňuje v hybridním systému s reverzní osmózou, kdy lze kapacitní deionizaci použít pro úpravu permeátu na odseparování zbylých iontů.

Kapacitní deionizace je založená na separaci nabitých iontů z roztoku elektrostatickými silami. Na láncích kapacitní deionizace probíhají faradaické a nefaradaické reakce, přičemž faradaické reakce jsou v kapacitní deionizaci nežádoucí, z důvodu oxidace elektrody, což snižuje účinnost separace. Samotný průběh adsorpce na elektrodu ovlivňuje celá řada faktorů: elektrodový materiál a jeho stáří, napětí, průtok, teplotu, pH, ionty obsažené v roztoku a počáteční koncentrace iontů.

V této práci byla použita jednotka kapacitní deionizace, kterou vyvinula firma ASIO, spol. s r. o. a cílem bylo optimalizovat vybrané faktory (napětí, průtok, vliv iontů obsažených v roztoku, vliv počáteční koncentrace iontů v roztoku a stáří elektrodového materiálu) a odzkoušet její účinnost na vybraných ukazatelích (vápenaté ionty, hořečnaté ionty, celková tvrdost, dusičnany, chloridy).

Zaměřili jsme se na selektivní účinnost odstranění iontů při procesu změkčování. Při experimentech u vybraných iontů došlo ke snížení koncentrace vápníku o 17,8 %, hořčíku o 54,2 % a u celkové tvrdosti vody došlo ke změkčení o 19,3 %. U aniontů došlo k poklesu obsahu dusičnanů o 46,2 % a u chloridů pouze o 16,2 %. Z výsledků je patrné, že metodu kapacitní deionizace lze použít pro separaci všech sledovaných iontů.

Literatura

[1] Daniel Weyessa Gari, František Kožíšek, *Zpráva o kvalitě pitné vody v ČR za rok 2020*, Státní zdravotní ústav, Praha, 2021

[2] Jakost vody. Brněnské vodárny a kanalizace [online]. Brno [cit. 2021-10-31]. Dostupné z: https://mapy.bvk.cz/jakost/

[3] P. Pitter, *Hydrochemie*, 2015, 792

Poděkování

Rád bych zde poděkoval firmě ASIO, spol. s r. o. za zapůjčení poloprovozní jednotky kapacitní deionizace pro experimentální část této práce.

Syntéza a charakterizácia spin crossover polymérnych systémov Hofmannovho typu s fotoizomerizovateľnými molekulami

Jana Vojčíková[1], Barbora Brachňáková[2], Lucie Routabol[3]

[1] Slovenská technická univerzita v Bratislave Fakulta chemickej a potravinárskej technológie Oddelenie anorganickej chémie

Radlinského 2101/9 812 37 Staré Mesto
jana.vojckova.13@gmail.com

[2] Slovenská technická univerzita v Bratislave Fakulta chemickej a potravinárskej technológie Oddelenie anorganickej chémie

Radlinského 2101/9 812 37 Staré Mesto

[3] Laboratoire de Chimie de Coordination (LCC) of the Centre National de la Recherche Scientifique (CNRS)

205 Route de Narbonne, 31400 Toulouse, Francúzsko

Cieľom tejto práce bola syntéza a charakterizácia poréznych trojdimenzionálnych koordinačných polymérov Hoffmanovho typu (ďalej už len MOF) s potenciálom vykazovať spin crossover efekt (ďalej už len SCO). Fyzikálna podstata týchto systémov je zaujímavá z hľadiska fotoindukovaného SCO, ktorý je riadený prítomnosťou - izomerizovateľných hosťujúcich molekúl, ktoré účinkom svetla podliehajú izomerizácií alebo cyklizácií v dôsledku čoho dochádza k zmene magnetických vlastností MOF systému (tzv. GD – LISC fenomén; z angl. Guest-Driven Light-Induced Spin Crossover).

Táto práca v prvom kroku nadväzuje na predošlý výskum vedeckej skupiny J.A Reala [1] a využíva klatrát {Fe(bpac)[Ni(CN]$_4$}, kde bpac =1,2-bis(4-pyridyl)acetylén. Dostatočne veľké póry nachádzajúce sa v štruktúre tohto klatrátu umožnili implementáciu hosťovských molekúl (antracén, fenantrén, cis-stilbén a trans-stilbén) a pomocou nich modifikovať magnetické a SCO vlastnosti pôvodného MOF systému. Dôvodom, prečo sme sa zamerali práve na tieto molekuly je skutočnosť, že fyzikálne vlastnosti MOF polymérov vieme ovplyvňovať pomocou svetla alebo teploty. Rozdielne SCO vlastnosti pripravených zlúčenín sú dôsledkom interakcií hosť-hostiteľ, čo súvisí so stérickými a elektronickými efektmi. Výsledky poukázali na to, že metóda prípravy úzko súvisí množstvom hostí v dutinách a teda priamo ovplyvňuje spinové vlastnosti. Ako najvhodnejšia metóda sa javí metóda priamej syntézy, pretože krivka závislosti magnetickej susceptibility od teploty je strmá s teplotnou hysteréziou, čo je žiadúce, ak takéto materiály majú byť využité pre aplikačné účely. Predpokladaný výsledok, to že SCO vlastnosti súvisia s povahou a množstvom hostí v dutinách nám potvrdili magnetické merania ako aj merania reflektivity. Pomocou nepriamych analytických metód ako elementárna analýza, infračervená spektroskopia s Fourierovou transformáciou a termogravimetria sme identifikovali zloženie nami pripravených systémov a potvrdili prítomnosť hostí v kavitách. Okrem potvrdenia prítomnosti hosťujúcich molekúl vložených do MOF sme zisťovali pomocou teplotne závislej Ramanovej a infračervenej spektroskopie aj informácie o konverznej krivke, teda či nami pripravené zlúčeniny vykazujú spinový prechod a pri akej teplote sa nachádza.

V konečnej fáze sme sa venovali experimentom s ožarovaním nami pripravených zlúčenín v roztoku za účelom „prepnutia“ trans-stilbénu na cisstilbén, následne prídavkom oxidačného činidla získať fenantrén a sledovať zmeny v magnetických vlastnostiach. Druhý experiment bol založený na dimerizácii antracénu vo vnútri 3D polyméru použitím elektromagnetického žiarenia vlnovej dĺžky

350 – 470 nm. Bohužiaľ ani v jednom prípade sa nám zatiaľ nepodarilo preukázať že došlo k fotoizomerizácii, resp. dimerizácii, čo pripisujeme slabej priepustnosti MOF systému pre svetlo.

Literatura

[1] V. Niel, J. M. Martinez-Agudo, M. C. Muñoz, A. B. Gaspar, J. A. Real, Inorg. Chem., 2001

Fyzikálno-chemická charakterizácia pyrolýznych materiálov na báze čistiarenských kalov

Diana Bošanská[1], Vladimír Frišták[1], Vladimír Turčan[1], Gerhard Soja[2]

[1] Katedra Chémie, Pedagogická fakulta, Trnavská univerzita

v Trnave, Priemyselná 4, Trnava, 917 01

[2] Institute of Chemical and Energy Engineering, University of Natural Resource and Life Sciences Vienna

Muthgasse 107, 1190 Vienna, Austria

Zhodnocovanie čistiarenských kalov je často limitované vysokým obsahom toxických foriem kontaminantov anorganickej ako aj organickej povahy. Jednou z možností ako efektívne spracovať vo svete neustále rastúce množstvá čistiarenských kalov je proces pyrolýzy. Termochemická konverzia čistiarenských kalov sa s pribúdajúcimi výskumnými prácami ukazuje ako sľubná metóda na spracovanie týchto heterogénnych a značne komplikovaných odpadov. Produkty pyrolýzy čistiarenských kalov majú kvôli variabilite fyzikálno-chemických vlastností a obsahu ťažkých kovov, ako aj organických polutantov obmedzené použitie [1]. Akokoľvek, prítomnosť ťažkých kovov, ktoré sa v procese pyrolýzy multiplikujú vo výslednom produkte, otvára otázky ohľadne ich biologickej prístupnosti a extrahovateľnosti [2].

Pyrolýzne upravený čistiarenský kal pripravený pri teplote 603-615°C sme charakterizovali pomocou stanovenia pH, EC, CHN-S-analýzou, celkového P, CAL-extrahovaného P, frakcionácie viazaných foriem fosforu v materiáli, stanovenia prítomnosti polycyklických aromatických uhľovodíkov (PAU), SEM-EDX analýzy povrchov. Skúmaný materiál bol podrobený ekotoxikologickým testom (*Daphnia pulex, Lepidium sativum*) a kultivačnému testu (*Raphanus sativus*). CHNS elementárnou analýzou bol zistený celkový obsah C (35,5%), H (0,95%), N (4,21%) a S (0,72%). Aktívne aj potenciálne pH pyrolýznej vzorky bolo v kyslej oblasti (pH_{H2O} = 6,4, pH_{KCl} = 5,73). Elektrická vodivosť pyrolýzneho materiálu bola 623,3 µS/cm. Obsah popola predstavoval 27,09% a obsah prchavých látok bol 6,57%. Celková koncentrácia fosforu bola stanovená na 60,23 mg/g a hodnota CAL extrahovateľného fosforu bola 7,25 mg/g. Sekvenčnou extrakciou sme zistili koncentrácie extrahovaného fosforu s dominantným zastúpením pomaly uvoľniteľných foriem fosforu (NaOH – extrahovateľný P). SEM-EDX analýza odhalila štruktúrne zmeny povrchov, ako aj pravdepodobné formy väzby P. Celkový obsah PAU predstavoval koncentráciu 1,054 mg/kg. Ekotoxikologické testy ukázali, že pyrolýzny materiál nemal negatívny vplyv na skúmané organizmy *Daphnia pulex a Lepidium sativum*. Krátkodobý kultivačný experiment poukazoval na signifikantný vplyv 10% prídavku pyrolýzneho materiálu na rast biomasy reďkovky siatej.

Na základe získaných výsledkov sa pyrolýzny materiál pripravený z komunálneho čistiarenského kalu zdá byť sľubným pôdnym aditívom a potenciálnou alternatívou konvenčných anorganických hnojív.

Literatúra

[1] Faria, W.M. a kol., in *Archives of Agronomy and Soil Science*, 2017, Vol. 64, p. 505-519.

[2] Frišták, V. a kol., in *Journal of Cleaner Production*, 2018, Vol. 172, p. 1772-1778.

Poďakovanie

Práca vznikla s finančnou podporou APVV projektu SK-AT-20-0004 „Pôdne aditíva na báze pyrolýznych materiálov pre stabilizáciu pôdnej organickej hmoty a recykláciu nutrične dôležitých látok.

SEKCE STUDENTŮ DOKTORSKÝCH PROGRAMŮ

1) Life Science - Sekce organické, environmentální chemie a biochemie

Self encapsulation of plant growth-promoting bacteria Azotobacter vinelandii for their use as next-generation bioinoculants

D. Černayová[1], M. Sukeník[1], P. Sedláček[1], S. Obruča[1]

[1] Faculty of Chemistry, Brno University of Technology, Brno, CZ

Purkyňova 464/118, 612 00 Brno

Azotobacter vinelandii is a plant-growth-promoting bacterium (PGPB), capable of synthesizing two different biopolymers with great application potential. Polyhydroxyalkanoates (PHA) are produced and stored in a form of intracellular granules, whereas alginate is produced extracellularly. Plant growth-promoting bacteria can be used as bio-inoculants to increase yields in agriculture. Encapsulation of bacteria into hydrogel-based carriers substantially improves the application potential of the bioinoculant as well as the viability and robustness of the bacterial culture. In this work, the alginate produced by the bacteria themselves was crosslinked with a calcium chloride solution to form a hydrogel carrier with encapsulated bacteria. This unconventional concept that we termed „self encapsulation“ simplifies bacterial encapsulation and production of hydrogel carriers, reduces the cost, and expands its usability in numerous applications. Firstly, we screened five strains of *Azotobacter vinelandii* to select those with a sufficient production capacity concerning alginate and PHA and suitable gelation properties. Actually, the strain DSM 87 reached the highest concentration of the alginate (4.9 ± 0.6 g/l). The alginates produced by strains DSM 87 and DSM 720 demonstrated the best gelation properties. The bacterial entrapped in a gel matrix seemed to be viable and cultivatable. Hence, the preliminary results confirmed the feasibility and viability of the novel concept.

Development of a Multiplex PCR Assay for Simultaneous Detection of Closely Related Fruit Species in Food

Lenka Fialová[1], Denisa Langová[1],
Adriana Prachárová[1], Ivana Márová[1]

[1] Brno University of Technology, Faculty of Chemistry

Purkyňova 464/118, 612 00 Brno
xcfialoval@vutbr.cz

Food adulteration is a long-standing problem. As new ways of adulteration develop, new methods for food authenticity checking, including DNA-based ones, should be developed, too. In this work we focused on multiplex real-time PCR-HRM and its possible use in simultaneous detection of various fruit species in food. New apricot-specific primers were also designed as a part of this work. Peach and apricot were chosen as the fruit species of interest because they occur as both the adulterant and the adulterated commodity [1], and because certain foodstuffs (such as infant food) contain both of these fruits. We analyzed three fruit purees, two of which contained approximately 70 % of apple and 30 % of either apricot or peach. In these purees, neither apricot nor peach was detected. The third puree contained both apricot and peach, but not apple. Using multiplex PCR, we were able to detect apricot in the last puree by both HRM analysis and electrophoresis, and peach was detected by electrophoresis. From these results we conclude that while multiplex PCR can be used for simultaneous detection of peach and apricot in certain foodstuffs, further study focusing on the influence of matrix type on the results of this method would be appropriate.

References

[1] Dasenaki, M.E.; Thomaidis, N.S. Quality and Authenticity Control of Fruit Juices-A Review. *Molecules* 2019, *24*, 1014. https://doi.org/10.3390/molecules24061014

Acknowledgement

This work was supported by project FCH-S-21-7483.

Environmental risk assessment of polyhydroxybutyrate micro-bioplastics – summary of project results

Jakub Fojt [1], Václav Pecina[1,2], Petra Procházková[1],
Tereza Hammerschmiedt[2], Jiří Holátko[2],
Pavla Denková[1], Ondřej Malíček[2], Antonín Kintl[2,3],
Martin Brnický[1,2], Jiří Kučerík1

[1] Brno University of Technology, Faculty of Chemistry, Institute of Chemistry and Technology of Environmental Protection

Purkyňova 118, 61200
xcfojt@fch.vut.cz

[2] Department of Agrochemistry, Soil Science, Microbiology and Plant Nutrition, Mendel University in Brno

Zemědělská 1, 613 00 Brno, Czech Republic

[3] Agriculture Research, Ltd.

Zahradni 400/1, 664 41 Troubsko, Czech Republic

Mankind invests significant amount of resources and effort to decrease micro-plastics production; one of the solutions is replacement the conventional plastics by biodegradable plastics. However, the conditions for biodegradation are not always met in real environment, thus the degradation of the bioplastics is slow or incomplete and paradoxically it leads to the micro-bioplastics formation [1]. The adverse ecotoxicological effects of conventional micro-plastics on living organisms are known, but the micro-bioplastics are almost overlooked [2]. There is also lack of articles describing the effect of both micro-plastics and micro-bioplastics on soil abiotic processes [3]. We tried to address this issue by analyzing the effect of polyhydroxybutyrate (PHB) micro-bioplastics and polyethyleneterephtalate (PET) microplastics. The aim was to assess I) the effects of PHB micro-bioplastics on soil structure, II) the effect of PHB on soil megafauna, and III) how the biodegradation of bioplastics effects the nutrient content, microbiological activity and thus the crops growth.

We used following setups. I) Influence of MPs on abiotic characteristics of soil was investigated in sapric histosol spiked with different concentrations of micro-plastics and micro-bioplastics exposed to the different relative humidity. The soil indicator describing the soil water retention and desiccation (water holding capacity and soil water evaporation enthalpy) and effects on soil structure were measured using DSC. II) The ecotoxicological adverse effects caused of PHB was tested according to the OECD acute, chronic and escape earthworm tests. The pot maize plant experiment was conducted to describe effects of PHB micro-bioplastics on the crops and agricultural soil. III) The maize seeds planted in pots were exposed to different concentrations of PHB. Subsequently the pots were kept in the growth chamber for 90 days and then the plants were harvested. The plant biomass, soil microbial activity and soil microorganisms were analyzed.

Results: We have found out that contamination of micro-plastics and micro-bioplastics results in changes in the soil organic matter structure and accelerated desiccation of soil. The presence of micro-bioplastics also leads to microbial activity boost, the mineral soil nutrient depletion, and significantly lower yields of biomass.

References

[1] Fojt, J.; David, J.; Přikryl, R.; Řezáčová, V.; Kučerík, J. A Critical Review of the Overlooked Challenge of Determining Micro-Bioplastics in Soil. *Science of the Total Environment,* 2020.

[2] Liwarska-Bizukojc E. 2021. Effect of (bio)plastics on soil environment: A review. *Science of The Total Environment*.

[3] de Souza Machado, A. A.; Kloas, W.; Zarfl, C.; Hempel, S.; Rillig, M. C. Microplastics as an Emerging Threat to Terrestrial Ecosystems. *Global Change Biology*. 2018.

Acknowledgement

The financial support of projects FCH-S-21-7398 and Kvalitní interní granty VUT EF19_073/0016948 of Ministry of Education, Youth and Sports are acknowledged.

Synthetic approaches towards novel vitamin B_2-inspired derivatives for organic (bio)electronics

Lucia Ivanová[1], Jan Richtár[2], Jozef Krajčovič[3]

[1] Brno University of Technology, Faculty of Chemistry
Purkyňova 118, 612 00 Brno, Czech Republic
xcivanova@vutbr.cz,

[2] Brno University of Technology, Faculty of Chemistry

[3] Brno University of Technology, Faculty of Chemistry
krajcovic@fch.vut.cz

The family of yellow pigments flavins includes nature-inspired molecules derived from the tricyclic heterocycle isoalloxazine. The omnipresent biological source, riboflavin, is an important segment of redox cofactors serving as electron shuttles within the cellular metabolism. Both natural and synthesised flavins share unique properties attributed to the isoalloxazine core, defining the redox and optical properties.

Our research group has recently studied the synthesizability of flavin derivatives resulting in the preparation of NH--free molecules with prolonged conjugation of the aromatic system [1]. In addition, we focused on the solubility of the molecules in common organic solvents and enhanced it by N,N'-alkylation, leading to better processability and consequent complex evaluation of the physicochemical properties [2].

The initial research served as a springboard towards constructing novel branched flavins with donor-π-donor (D-π-D) character. Thus, corresponding nature-inspired D-π-D systems are auspicious for the use in organic electronic and bioelectronic devices in terms of their biocompatibility, non-toxicity with a potential low-cost production. Herein, our current progress in synthesis is presented. The approach requires elaboration of a reliable method for preparing the responding 1,2-diketones to form the isoalloxazine core of the flavin by condensation reaction with 5,6-diaminouracil.

References

[1] J. Richtar, P. Heinrichova, D. Apaydin, V. Schmiedova, C. Yumusak, A. Kovalenko, M. Weiter, N.S. Sariciftci, J. Krajcovic, *Molecules* 23(9) (2018) 2271.
[2] J. Richtar, L. Ivanova, D.R. Whang, C. Yumusak, D. Wielend, M.Weiter, M.C. Scharber, A. Kovalenko, N.S. Sariciftci, J. Krajcovic, *Molecules* 26(1) (2021) 27.

Acknowledgement

The research was supported by the project 21-01057S funded by the Czech Science Foundation.

Biosource materials for coatings

Ing. Vojtěch Jašek

Vysoké učení technické v Brně, Fakulta chemická
Purkyňova 118, 612 00 Brno, Czech Republic
xcjasekv@vutbr.cz

The presentation is focused on the chemical processes leading to the production of polymerizable material precursors made out of the natural sources. There are various biosource substrates which can be transformed into the potential coating materials such as vegetable oils, sorbitol or lactic acid. The modification of these reactants via the acrylic acid, the methacrylic acid and the methacrylic anhydride has been studied. The aim of the further research is to invent new materials, which can combine positive properties of the material precursors, which have already been prepared. Modified vegetable oil structure contains a significant amount of biosource carbon. The sorbitol material precursor derivatives show high glass transition temperature numbers (T_g) after their polymerization. All these material are supposed to be an alternative to the materials used currently like pure acrylates or artificial polyurethanes.

Determination of carotenoids in vegetables by HPLC-DAD

Ing. Aliaksandra Kharoshka[1], Bc. Michaela Schreibmeierová, assoc. prof. Věra Schulzová, PhD

[1,2,3] University of Chemistry and Technology Prague, Faculty of Food and Biochemical Technology, Department of Food Analysis and Nutrition

Technická 3, 166 28 Prague 6, Czech Republic
kharosha@vscht.cz

Carotenoids are bioactive compounds that are widely found in nature as natural pigments, synthesised mostly by plants, algae and microorganisms. The main dietary sources of carotenoids are vegetables and fruits. Analysis of these compounds can be challenging because carotenoids are usually structural isomers or differ just in the number of hydroxyl groups. Liquid chromatography coupled with diode array detector or mass spectrometer are the most popular analytical techniques combinations used for the analysis [1,2].

Presented study focuses on quantitative determination of three major carotenoids – lutein, lycopene and β-carotene – using high performance liquid chromatography with diode array detection (HPLC-DAD). Overall, several varieties of fresh and frozen spinach, green peas, carrots, tomatoes and corn were analysed. These vegetables were chosen because they are rich in carotenoids. Analytes were extracted with and without hydrolysis. Separation was achieved using reverse phase C18 column with gradient elution. The eluent was further analysed at the characteristic detection wavelength for each carotenoid. The identification was based on comparison of the retention times and spectra of the measured samples with the standards. Quantification was done using external calibration. To ensure the precision of the method, certified reference material (CRM) was also analysed by the same method.

It was found that the crucial step was the alkaline hydrolysis as almost no free forms of carotenoids were detected. Also, there was nearly no difference between fresh and frozen vegetables in terms of carotenoids content. Such information can be important for food producers. The analysis of CRM showed that the method used is precise and reliable.

References

[1] R.K. Saini, S.H. Nile, S.W. Park, *Food Research International* 76 (2015): 735-750.
[2]K. T. Amorim-Carrilho, A. Cepeda, C. Fente, P,Regal, *TrAC Trends in Analytical Chemistry* 56 (2014): 49-73.

Acknowledgement

This work was supported from the grants of Specific university research – grants No A2_FPBT_2021_033 and A1_FPBT_2021_001.

Utilization of waste material from wine production as a binding agent in DGT technique for heavy metals analysis in aquatic systems

Jakub Křikala[1], Pavel Diviš[1]

1 Brno University of Technology, Faculty of Chemistry, Institute of Food Chemistry and Biotechnology

Purkyňova 464/118, 612 00 Brno, Czech Republic
Jakub.Krikala@vut.cz

The diffusive gradients in thin films technique (DGT) was first reported by Zhang and Davison in 1994 for determination of zinc in seawater. The DGT devices conventionally employs a diffusive layer consisting of polyacrylamide or agarose hydrogel, sorption layer consisting of appropriate binding agent immobilized in hydrogel and membrane filter as a protective layer. The principle of DGT technique is based on kinetic separation of metal ions, dissolved inorganic or small labile organic complexes from aquatic system according to Fick's First Law and their accumulation in sorption layer. A major advantage of DGT technique is the *in situ* deployment for metal bioavailability and time-integrated measurements. In addition, DGT preconcentrates metal solutes improving problems of contamination and method detection limits. Traditional DGT device for metal analysis comprise a Chelex-100 as binding agent, which can be used for the determination of 24 cationic metals. But for greater comprehensiveness of DGT, many other materials have been employed as adsorbents due to their availability or selectivity for specific chemical species. One way of the recent research progress of DGT technique is utilization of low-cost materials an agricultural by-products as binding agents considering an economic and green-technology approach. For example, banana peels, coffee grounds or baker's yeast have already been used in DGT technique for metal ions determination [1-3].

This study focuses on using of waste material from wine production as possible binding agent in DGT technique. High content of organic matter makes wine-processing waste material an excellent sorbent for removing metal ions from aquatic system because of high content of functional groups (such as carboxylic or phenolic compounds) present in the cell wall of the material. These compounds provide attractions forces to the metal causes their high-efficiency removal. First step of experimental part was preparation of material and its incorporation into agarose hydrogel to prepare binding layer. Wine waste and agarose-waste gel disks were characterized by Scanning Electron Microscopy, Energy Dispersive X-ray Spectrometry and IR spectroscopy. In order to study the binding kinetic and uptake efficiency of metal ions, the agarose-waste gel disks were deployed in 50 ml of a 1 mg.l^{-1} of mixed metal solution (0.05M NaNO3 at pH 5,5±0,1) under constant stirring for 48 hours in triplicate, whereas in different time intervals subsamples were taken for ICP-OES analysis. To assess the elution efficiency the agarose-waste disks were put into 50 ml of a 1 mg.l^{-1} of metal solution under the same conditions. 1M HNO_3 and 2M HCl were used as elution agents. This study has shown good selectivity of wine waste incorporated in agarose hydrogel for Al, Cr, Cu, Fe and Pb determination from aqueous solutions in laboratory deployment, so next experiments with bioadsorbents will be performed.

References

[1] W. Davison, H. Zhang, Nature 367 (1994) 546-548.

[2] L.N. Marques Yabuki, K.S. Luko Sulato, M.R. Boniolo, A.A. Menegário, M.L. Garcia, International Journal of Environmental Analytical Chemistry 1-25

[3] L.N.M. Yabuki, A.A. Menegário, H. Gemeiner, A.M.C.M. Rolisola, D. Gastmans, P.M. Williams, Talanta 205

ISOLATION OF FERULIC ACID FROM WHEAT BRAN HYDROLYZATE BY ADSORPTION

Jakub Nábělek [1], Jaromír Pořízka[1], Pavel Diviš1

[1] Brno university of technology, faculty of chemistry

Purkyňova 464/118, 612 00 Brno
xcnabelek@vutbr.cz

Together with maize and rice, wheat accounts for about 90 % of the world's cereal production. Besides other valuable compounds such as wheat germ and endosperm parts, wheat bran remains a major by-product during the milling process [1]. Wheat processing mills can produce up to 50 tons of bran per day. This waste material is suitable for further processing, as it still contains a significant proportion of phenolic compounds, especially ferulic acid. Ferulic acid is contained in bran in the form of feruloylated oligosaccharides [2].

The aim of this work was to develop a method for the isolation of ferulic acid from wheat bran. The research was divided into several segments. The first part of this work was focused on the pre-treatment of wheat bran. Wheat bran was subjected to protein removal to increase the purity of the final product.

The next step in the process was to obtain the wheat bran hydrolysate to release ferulic acid into the solution. This step was realized by alkaline hydrolysis. This process was modified from the process described by Buranov [3]. Hydrolysis of bran was performed by 0,5 M NaOH in stirred, heated reactor with reaction time 4 hours at 50 °C with mixing at 180 rpm. After reaction, the solution was adjusted by the addition of 3M HCl to pH 3. A solid part of the mixture was separated by centrifugation.

Supernatant after hydrolysis was subjected to isolation of ferulic acid by adsorption on amberlite XAD-16. The ratio of adsorbent to supernatant was 1 g to 150 ml. Adsorption was performed at pH 3 for 50 minutes with continuous stirring. Supernatant and adsorbent were further separated by 0,1 mm sieve. The adsorbent was rinsed by a solution of HCl with pH 3.

Desorption of ferulic was the final step. It was made by mixing the adsorbent with 96% ethanol. Desorption was performed at laboratory temperature for 60 minutes with continued stirring at 150 rpm.

Analysis of isolate was carried out by reversed phase HPLC on Shimadzu SCL-10 A with Kinetex 2.6 μm; C18; 100 × 4.60 mm column with 10 % acetonitrile and 90 % acetic acid (1% v/v) mobile phase.

Based on the analyses, the efficiency of the whole process was evaluated. The amount of ferulic acid in the final isolate solution was 676 ± 57 mg/l. This is equal to yield 1,38 ± 0,27 g/kg ferulic acid from deproteinate wheat bran. The isolate does not contain only ferulic acid and solvent. The isolate can contain a variety of substances such as polysaccharides, proteins, salts or other phenolic substances. The main contaminant was identified as proteins (4,38 ± 1,16 g/l).

References

[1] Prückler, M., Siebenhandl-Ehn, S., Apprich, S., Höltinger, S., Haas, C., Schmid, E., & Kneifel, W. (2014). Wheat bran-based biorefinery 1: Composition of wheat bran and strategies of functionalization. LWT - Food Science and Technology, 56(2), 211-221. https://doi.org/10.1016/j.lwt.2013. 12. 004

[2]KIM, K., TSAO, R., YANG, R., & CUI, S. (2006). Phenolic acid profiles and antioxidant activities of wheat bran extracts and the effect of hydrolysis conditions. Food Chemistry, 95(3), 466-473. https://doi.org/10.1016/j.foodchem.2005. 01. 032

[3]Buranov, A. U., & Mazza, G. (2009). Extraction and purification of ferulic acid from flax shives, wheat and corn bran by alkaline hydrolysis and pressurised solvents. Food Chemistry, 115(4), 1542-1548. https://doi.org/10.1016/j.foodchem.2009. 01. 059

Influence of Bioplastics' Biodegradation on Soil Quality

Natálie Paluchová[1], Jiří Kučerík[2]

[1] Brno University of Technology, Institute of Chemistry and Technology of Environmental Protection

Purkyňova 464, Brno, 612 00
Natalie.Paluchova@vut.cz

[2] Brno University of Technology, Institute of Chemistry and Technology of Environmental Protection

Over the past decade, the society has brought attention to microplastics. They are produced by various industries and spread across the environment. As they are no longer considered inert (with no further effects on plants and other living organisms) many researchers including us are constantly working to address this situation. In this sense, bioplastics has been brought to a media spotlight. They are presented as an ecological alternative to solve generally plastic related problems, but what is often forgotten, their main advantage might also be their bottleneck.

Majority of scientific articles, focusing on their presence in the environment are limited only on marine and fresh waters [1] and therefore their behaviour in air and soil remains rather unclear. For that reason, a work mentioned in this contribution focuses on negative effects associated with presence of microplastics (specifically poly-(R)-3-hydroxybutyrate bioplastic) in soils as their common receptor. We consider soil to be a recycling facility - carbon is circulated to the atmosphere as carbon dioxide, nitrogen is made available as ammonium and nitrate, and the rest of the associated elements appear in forms required by higher plants [2]. In this sense, during microbial decomposition of carbon-rich compounds, only part of the carbon is released, and the rest remains in the form of soil organic matter. This matter is available to all living organisms and is being constantly reused. Addition of any substrate (in our case a bioplastic) to such an environment will cause an imbalance in this system, which can seriously endanger soil quality and thus plants and living organisms. Therefore, it is essential to focus on their transport and transformation in the environment.

To investigate physico-chemical changes in soil induced by the presence of bioplastic, we combined respirometry, elemental analysis, thermogravimetry and enzymatic assays. Our results suggested a negative effect on soil organic matter and water retention in soil. A phenomenon called „priming effect“ [3] was widely investigated as acceleration as well as retardation of soil organic matter decomposition took place. We registered different influence of selected concentrations of biopolymer on the soil system as well as an influence of soil properties on the course of degradation. Finally, increased enzymatic activities clearly suggested impact of biopolymer presence on the microbial community. Such findings let us conclude, that biopolymer addition leads to long-term impact on a range of soil ecosystem services.

References

[1] ISSAC, M.N. a B. KANDASUBRAMANIAN. Effect of microplastics in water and aquatic systems. *Environmental Science and Pollution Research*. Springer, 2021, **28**(16), 19544–19562. Available from : https://doi.org/10.1007/s11356-021-13184-2

[2] STEVENSON, F. J. a M. A. COLE. *Cycles of Soils: Carbon, Nitrogen, Phosphorus, Sulfur, Micronutrients, 2nd Edition*. 2. New York: Wiley, 1999. ISBN 978-0-471-32071-5.

[3] BLAGODATSKAYA, E. a Y. KUZYAKOV. Priming Effects in Relation to Soil Conditions – Mechanisms. GLIŃSKI, J., J. HORABIK a J. LIPIEC*. Earth and Environmental Science Reference Module Physical and Materials Science: Encyclopedia of Agrophysics* [online]. Dordrecht: Springer, 2011, s. 657-667 [cit. 2021-11-11]. ISBN 978-90-481-3585-1. Available from : https://doi.org/10.1007/978-90-481-3585-1_128

Contamination of Urban Forest Soils with Potentially Toxic Elements in Brno City, Czech Republic

Václav Pecina[1], David Juřička[2], Jitka Hegrová[3], Martin Brtnický[1], Renata Komendová[1]

[1] Brno University of Technology, Faculty of Chemistry, Institute of Chemistry and Technology of Environmental Protection

Purkyňova 118, 612 00 Brno, Czech Republic
xcpecina@fch.vut.cz

[2] Mendel University in Brno, Faculty of Forestry and Wood Technology, Department of Geology and Soil Science

Zemědělská 3, 613 00 Brno, Czech Republic

[3] Transport Research Centre

Líšeňská 33a, 636 00 Brno, Czech Republic

Urban forests are an important component of urban ecosystems, given many beneficial services they provide. The quality of the services, however, can be adversely affected by a soil contamination with potentially toxic elements. Despite the high research interest in the contamination of urban soils, the contamination of forest soils in cities remains on a fringe of a scientific interest. The aim of this study was to assess the contamination of urban forest topsoil (0–10 cm) with potentially toxic elements in Brno City, Czech Republic. A total of 50 soil samples were taken and analysed using the triple quadrupole inductively coupled plasma mass spectrometer (ICP-MS/MS) after a decomposition in *aqua regia*. Results were

compared with limits from the Czech Decree No. 153/2016 Coll. on agricultural soil quality. The median values for As, Cd, Cr, Cu, Ni, Pb and Zn were 7.98, 0.22, 30.1, 15.2, 12.3, 25.4 and 62.7 mg/kg, respectively. The limits were exceeded for Cd, Cu, Ni, Pb and Zn in 8, 6, 4, 2 and 16% of cases, respectively. The limits for As and Cr were not exceeded. The results suggested that the contamination of forest soils in Brno is predominantly low. However, the contamination found can potentially adversely affect quality of forest products, such as mushrooms, and local forest ecosystem services.

Assessment of the effect of pasteurization and filtration on the content of selected nutrients in beer

Lenka Punčochářová[1], Jaromír Pořízka[2], Pavel Diviš[2], Adéla Šimíčková, Dominika Vopelková, Václav Štursa

1 Brno University of Technology, Faculty of Chemistry, Department of Food Chemistry and Biotechnologies

Purkyňova 118, 612 00 Brno, Czech Republic
xcpuncocharoval@fch.vut.cz

2 Brno University of Technology, Faculty of Chemistry, Department of Food Chemistry and Biotechnologies

Purkyňova 118, 612 00 Brno, Czech Republic

Beer is a complex chemical matrix that consists of over 450 constituents [1]. Besides polysaccharides, proteins, lipids and organic acids beer also contains nutritionally important substances such as vitamins, phenolic compounds and elements [2]. Phenolic compounds affect the formation of beer haze, redox state, colour, flavour, foam stability and stability of the beer during aging [3]. Mineral content is significantly connected to sensory properties of beer, enzymatic activity during mashing and regulate processes during boiling, cooling and fermentation of wort [4]. B vitamins are water-soluble substances used by yeasts in many biochemical pathways as cofactors. Post-fermentation treatments (e.g. pasteurization, filtration) are important in brewing to achieve stability and durability of the final product and form desired organoleptic properties. However, these procedures may influence the chemical composition of beer [5].

In this study, a total of 28 samples of beer were analysed. They were divided into three groups according to their post-fermentation treatments – NPNF (non-pasteurized, non-filtered), NPF (non--pasteurized, filtered) and PF (pasteurized, filtered). The content of catechin, gallic acid, vanillic acid, coumaric acid, ferulic acid and B group vitamins (B2, B3, B6, B9 and B12) were determined using HPLC-DAD. Elemental analysis of beer was performed by ICP-OES. This research indicates that post-fermentation treatments affect the chemical composition of beer and its nutritional value. Pasteurization and filtration caused a decrease of phenolic compounds content. Filtration influenced concentration of riboflavin and niacin. Another statistically significant differences were identified in the content of elements, specifically Fe, K, Si and Mg.

References

[1] Brewing: Science and practice. D. E. Briggs, C. A. Boulton, P. A. Brookes, R. Stevens (Eds.), Cambridge, Woodhead Publishing, 2004.

[2] F. Vivian, C. T. Aoyagui, D. Noin De Oliveira, R. R. Catharino, Mass spectrometry for the characterization of brewing process, Food Research International, 2016, 281-288.

[3] D. Šibalić, M. Planinić, A. Jurić, A. Bucić-Kojić, M. Tišma, Analysis of phenolic compounds in beer: from raw materials to the final product, Chemical Papers, 2021, 67–76.

[4] A. A. D. Comrie, Brewing liquor – a review, Journal of The Institute of Brewing, 1967, 335-346.

[5] B. Hucker, F. Vriesekoop, A. Vriesekoop-Beswick, L. Wakeling, H. Vriesekoop-Beswick, A. Hucker, Vitamins in brewing: effects of post-fermentation treatments and exposure and maturation on the thiamine and riboflavin vitamer content of beer, Journal of The Institute of Brewing, 2016, 278-288.

Acknowledgement

This work was supported by the Ministry of Education, Youth and Sports of the Czech Republic, grant no. FCH-S-21-7483.

NUTRITION PROPERTIES OF WHEAT BRAN PROTEIN ISOLATES

Zuzana Slavíková[1], Jaromír Pořízka[1],
Jakub Nábělek[1], Pavel Diviš[1]

[1] Brno University of Technology, Faculty of Chemistry,
Department of Food Chemistry and Biotechnologies

Purkyňova 464/118, 612 00, Brno, Czech Republic
zuzana.slavikova@vut.cz

Proteins are one of the most important group of nutrients, they should contribute to about 10–35 % of the human diet. However, in modern lifestyles, people don't have enough time to intake a sufficient amount of proteins. Fortification of food by proteins is a solution to protein deficiency in the diet. The food can be fortified by animal or plant proteins, which differ in nutrition properties, but also in price. Plant sources of proteins are cheaper and, therefore, more available also for the ordinary people. Wheat bran is one of the significant plant source of proteins. It is a secondary product of wheat utilization and contains approximately 16 % of proteins. About 50 % of the wheat bran proteins are not digestible, as they are part of complicated polysaccharide structures.

Experiments were focused on the development of the protein isolation method. The digestible protein fraction was successfully isolated from wheat bran by pH-shift method. After an alkaline extraction and centrifugation of raw wheat bran, proteins were released to the supernatant. These proteins were then precipitated by adjustment to pH 4. The yield of the isolation process was about 8 % with 90% protein content. Dehydration of the product was performed by lyophilization.

Isolated protein material was subjected to chemical characterization. After lyophilization, the isolated material contained about 8 % of water. Based on the amino acid analysis, it was found, that the most abundant amino acid is arginine, which is important to e.g. for muscles growth and regeneration. Minor components of the isolated material are ferulic acid, which is a very good antioxidant, and glucose, whose content was up to 0,5 %. One of the important characteristics of this material is its mineral content. ICP-OES analysis of the isolated material has shown that it contains only 337 ± 3 mg/kg phosphorus. According to the phosphorus/protein ratio, this material seems to be suitable for the nutrition of people with kidney diseases.

Acknowledgement
The presented work was financially supported by project FCH-S-21-7483 (The Ministry of Education, Youth and Sports of the Czech Republic).

3D Scaffolds Based on Bacterial Cellulose

Radim Stříž[1], Nicole Černeková[1], Jiří Smilek[2], Falk Liebner[3], Patrycja Bober[4], Adriana Kovalcik[1]

[1] Brno University of Technology, Faculty of Chemistry, Institute of Food Chemistry and Biotechnology

Purkynova 118, 612 00 Brno, Czech Republic
Radim.Striz@vut.cz

[2] Brno University of Technology, Faculty of Chemistry, Institute of Physical and Applied Chemistry

[3] University of Natural Resources and Life Sciences, Vienna, Div Chem Renewable Resources

[4] Institute of Macromolecular Chemistry, Department of Conductive Polymers, Czech Academy of Sciences

Bacterial cellulose is an extracellular polysaccharide formed as a protective envelope around certain types of bacterial cells. The application of bacterial cellulose has been explored in many areas, such as the food industry, medicine, biotechnology, cosmetics, electronics, and textile industry. Several cultivation methods have been investigated to enhance bacterial cellulose production and decrease its cultivation costs [1].
This work involves optimizing bacterial cellulose by modifying the production medium and subsequently preparing 3D samples of bacterial cellulose to increase its mechanical stability.

It has been found that an increase in bacterial cellulose production can be achieved by modifying the surface of the gas-liquid interface, such as by aeration, the addition of acetate buffer, or oil. Active aeration increased bacterial cellulose production by 235%. Next, the effect of using fed-batch cultivation compared to static batch cultivation was also verified.

In this work, several cultivation strategies have been employed to produce stable mechanical 3D bacterial cellulose scaffolds in-situ during the cultivation of *Komagateibacter xylinus*. The most effective methodologies enabling bacterial cellulose production in the form of cylinders with a height of up to 2 cm were: 1) the static cultivation of *K. xylinus* inside the stable foam [2] or 2) cultivation in Hestrin-Scharmm medium with the addition of polyvinyl alcohol. The morphological investigations have shown that the bacterial cellulose's porosity varies significantly depending on the applied cultivation methodology.

It can be concluded that porosity is an important parameter that affects the absorption of water and the viscoelastic properties of bacterial cellulose scaffolds. The advantage of scaffolds with variable porosity based on bacterial cellulose is their non-toxicity, biocompatibility and the possibility of gradual release of the bioactive substance or drug.

References

[1] J. Wang, J. Tavakoli, Y. Tang, Bacterial cellulose production, properties and applications with different culture methods – A review, Carbohydrate Polymers 219 (2019) 63-76.

[2] P.A. Rühs, F. Storz, Y.A.L. Gómez, M. Haug, P. Fischer, 3D bacterial cellulose biofilms formed by foam templating, npj Biofilms and Microbiomes 4(1) (2018) 1-6.

Acknowledgement

This work was supported by the Ministry of Education, Youth and Sport of the Czech Republic (project No. 7AMB19AT) and the Austrian Agency for International Cooperation in Education and Research (OeAD-GmbH) (project No. WTZ 12/2019). Next, this work was funded through the Internal Brno University of Technology project FCH-S-21-7483.

Wastewater preconcentration method for the determination of legislation limits of cadmium, arsenic, zinc, copper, nickel, chromium and lead employing portable ED-XRF

Jiří Sýkora [1], Renata Komendová[2]

[1] Brno University of Technology, Faculty of Chemistry,
Department of Chemistry and Technology of Environmental
Protection

xcsykoraj@vutbr.cz

[2] Brno University of Technology, Faculty of Chemistry,
Department of Chemistry and Technology of Environmental
Protection

The chemical laboratories of the Fire Rescue Service of the Czech Republic (hereinafter referred to as CHL FRS) encounter the issue of determining hazardous metals in wastewater or surface water several times a year. The determination of hazardous metals such as arsenic, copper, lead, zinc, chromium, nickel or cadmium can be problematic, since not all CHL FRS have available instrumentation infrastructure such as ICP-OES or ICP-MS, for determination of trace amounts of heavy metals in samples. However, all CHL FRS have a mobile energy-dispersive X-ray fluorescence analyzer Delta X (hereinafter ED-XRF). The detection limits of ED-XRF for above-mentioned elements are at a concentration level of 10 mg/l. The limits for selected elements in the surface water and wastewater are specified in Government Regulation No. 401/2015 Coll. from

tenths to several mg /l If CHL FRS are to achieve these values by ED-XRF, it is necessary to use an effective preconcentration technique.

Keywords
Cd, As, Zn, Cu, Ni, Cr, Pb, ED-XRF, preconcentration, wastewater.

Acknowledgement
This study was supported by the Ministry of Education, Youth and Sports of the Czech Republic, fund No. FCH-S-21-7398.

The Effect of Feed Composition On the Metabolome of Edible Insects

Kateřina Šebelová[1], Jana Hajšlová[1]

[1] University of Chemistry and Technology in Prague, Faculty of Food and Biochemical Technology, Department of Food Analysis and Nutrition

Technická 5, 166 28 Prague 6, Czech Republic
sebelovk@vscht.cz

The world population is constantly growing thus the demands for food crops are increasing. [1] This puts enormous pressure on food systems. One of the solutions how to supply the population with enough nutrients and especially proteins is the production of edible insects. In comparison with the common livestock, insects grow faster and the conversion of the feed is fairly higher. Moreover, edible insects farming produces less greenhouse gas, leaves a smaller environmental footprint, and demands on water and space are also lower. [2] These advantages make edible insects a possible challenging sustainable alternative to traditional animal protein sources and make it a possible future common ingredient of food and feed. This potential usage of insects makes this commodity a growing concept and draws the attention of researchers who mainly focus on the impact of rearing conditions such as temperature on biomass gain, feed conversion, and nutritional properties. [3,4] However, there is still a lack of information on the effect of the feed composition on the content of bioactive substances, both desirable and undesirable, which affect the resulting safety and quality of edible insects.

This study we focused on the evaluation of the impact of rapeseed meal added to feed on the composition and quality of the Jamaican field cricket (*Gryllus assimillis)* biomass. For this purpose, metabolomic analysis using ultra-performance liquid chromatography with high-resolution tandem mass spectrometric detection (U-HPLC–HRMS/MS) was chosen as a suitable approach. Using the subsequent multivariate statistical analysis, it was possible to distinguish the tested groups of the Jamaican field crickets according to the composition of the feed. In addition to that, thiamine and sinapine were evaluated as possible markers of the presence of rapeseed meal in the feed fed to the crickets. In addition to that, screening of goitrin in tested samples was carried out. This antinutrient of the rapeseed meal was not detected in any of the analyzed samples.

References

[1] FAO AND THE GEF: PARTNERS IN ACTION. Feeding people, protecting the planet. Food and agriculture organization of the United nations (FAO), 2018

[2] D. DOBERMANN, et al. *Nutrition Bulletin*, 42(4),2017, 293-308

[3] J.D. BJØRGE, et al. *Journal of Insect Physiology*, 107, 2018, 89-96.

[4] MORALES-RAMOS, JA. a ROJAS, MG. *Journal of Economic Entomology*, 108(5), 2015, 2259-2267.

Acknowledgement

This work was supported from the grant of Specific university research – grant A2_FPBT_2021_053, This work was supported by the OPPC (CZ.2.16/3. 1. 00/21537 and CZ.2.16/3. 1. 00/24503), NPU I LO1601, METROFOOD-CZ (MEYS Grant No: LM2018100)

SEQUENTIAL CHEMICAL FRACTIONATION AS A TOOL FOR ACCESSING THE ORGANIC MATTER IN BIOCHAR

David Sirucek[1], Michal Kalina[1], Martina Klučáková[1]

[1] Brno University of Technology, Faculty of Chemistry

Purkynova 118/464, 612 00, Brno, Czech Republic
davidsirucek@seznam.cz

This contribution is focused on utilization of a sequential chemical fractionation method for determination of organic matter content, its distribution in biochar and the possible use of biochar as a soil conditioner in agriculture. For these purposes the optimized chemical fractionation procedure was used to reveal the content of organic matter in different biochar samples with different properties (samples with European biochar certification for usage in agriculture) which depend significantly on the temperature used during a pyrolysis of biomass residues in the process of biochar production. In parallel, these samples were also fractionated by classic alkaline extraction to obtain the so-called extractable fraction of organic matter (NOM).

Biochar is one of the important soil conditioners, known for having positive effect on crop yield, soil quality, nutrient cycle and carbon sequestration due to the transfer of organic carbon from it to the soil. However, the effect depends on the properties of the biochar, its doses to the soil, but also on the properties of the soil itself. Surprisingly, some authors point to the fact that biochar does not always have a positive effect on soil, plants or microfauna. Therefore, it is necessary to perform its depth characterization to be able to predicts its role in soil and its optimal application dose [1].

Individual fractions obtained from sequential chemical fractionation as well as NOM samples were characterized by methods of elemental analysis (determination of organic elements content), thermogravimetry (contents of ash, organic matter and moisture). The results showed that the method of sequential chemical fractionation gives higher yields of organic matter compared to classical alkaline extraction. Moreover, the obtained fractions divided according to solubility and strength of binding to residual inorganic matter of biochar can be better characterized by physical-chemical methods, which provides more detailed information about organic matter in biochar and its possible effect on soil properties [2,3].

References

[1] TAN, Zhongxin, Carol S.K. LIN, Xiaoyan JI a Thomas J. RAINEY. Returning biochar to fields: A review. Applied Soil Ecology. 2017, 116, 1-11. DOI: 10.1016/j.apsoil.2017. 03. 017. ISSN 09291393.

[2] NEBBIOSO, A., PICCOLO, A. Basis of a Humeomics Science: Chemical Fractionation and Molecular Characterization of Humic Biosuprastructures. Biomacromolecules. 2011, 12(4), 1187-1199 [cit. 2019-03-31].

[3] *ŠIRŮČEK, David, Michal KALINA a Martina KLUČÁKOVÁ. Influence of the Application of lignite on the distribution of organic carbon in soil. In: ŠIRŮČEK, David, Michal KALINA a Martina KLUČÁKOVÁ. NANOCON 2020 12th International Conference on Nanomaterials - Research and Application. Ostrava: TANGER, 2021, 2020, s. 489-494. ISBN 978-80-87294-98-7. ISSN 2694-930X. Dostupné z: doi:10.37904/nanocon.2020.3765*

Acknowledgement

This work has been supported by project GJ20-28208Y from Czech Science Foundation of the Czech Republic.

SEKCE STUDENTŮ DOKTORSKÝCH PROGRAMŮ

2) Material Science - Sekce analytické, anorganické a materiálové chemie

Preparation and characterization of photocatalytic active thin layers of Tungsten Oxide via „Brick and Mortar“ method

Ing. Radim Bartoš [1], doc. Ing. Petr Dzik, Ph.D.[2]

[1] Institute of Physical and Applied Chemistry, Faculty of chemistry, Brno University of Technology

Purkyňova 464/118, 612 00 Brno
xcbarosr@fch.vutbr.cz

[2] Institute of Physical and Applied Chemistry, Faculty of chemistry, Brno University of Technology

Purkyňova 464/118, 612 00 Brno

Water treatment and pollutant degradation became aim of research these days and photocatalytic reactions provides promising results for this application. Most common catalyst for these applications is titanium dioxide. This compound has bandgap varied about 3,2 eV [1] which corresponds to UV light wavelength.

As alternative tungsten trioxide can be used. In comparison with titanium dioxide, bandgap is lower, 2.6 eV [2] which correspond to visible light (≈466 nm).

Suspension of Tungsten Oxide was prepared using powder of tungsten oxide and alcohol solution of acetylperoxotungstic acid (APTA). APTA was used as functional binder „mortar“ for deposition on glass substrate or FTO glass plates. Nanoparticles of tungsten oxide served as „brick“.

Acetylperoxotungstic acid was synthetized by dissolving tungsten powder in 30% hydrogen peroxide solution to form solution of peroxotungstic acid. The solution was filtered and added to glacial acetic acid. Final mixture was refluxed and vacuum dried. Yellowish flake powder of acetylperoxotungstic acid was formed. [3]

Prepared precursor suspension was ink-jet printed on Na-Ca glass and FTO glass plates in 1-5 layers. Samples were calcined in various temperature 200 – 500 °C.

Profilometry measurement showed mostly linear increase of layer thickness depends on number of deposition layers varied between 250 – 900 nm thickness.

Dependence of thickness, resp. photocurrent generation on calcination temperature was measured using profilometry resp. chopped linear voltammetry method. Thickness of samples was not dependent on calcination temperature. Photocurrent increased slightly with higher temperature until 400 °C and then started to drop at temperature over 400 °C.

During voltammetry was observed change of color of samples between voltage of 0,25 – 0,75 V. Voltammetry data corresponds with that occurrence with wide curve in that region. In this region layer was reduced and change of color occurred. With increasing voltage over 0,8 V layer undergoes re-oxidation and starts to react to chopped irradiance of light and generate photocurrent. Maximum of generated photocurrent of 1 cm^2 sample (300 μA) was observed between 1,5 – 2 V.

References

[1] SVOBODA, Tomáš, Michal VESELÝ, Radim BARTOŠ, Tomáš HOMOLA a Petr DZIK. Low-Temperature Mineralisation of Titania-Siloxane Composite Layers. *Catalysts*. 2021, **11**(1). ISSN 2073-4344. Dostupné z: doi:10.3390/catal11010050.

[2] GILLET, M., K. AGUIR, C. LEMIRE, E. GILLET a K. SCHIERBAUM. The structure and electrical conductivity of vacuum-annealed WO3 thin films. *Thin Solid Films*. 2004, **467**(1-2), 239-246. ISSN 00406090. Dostupné z: doi:10.1016/j.tsf.2004. 04. 018.

[3] DEEPA, M., T.K. SAXENA, D.P. SINGH, K.N. SOOD a S.A. AGNIHOTRY. Spin coated versus dip coated electrochromic tungsten oxide films: Structure, morphology, optical and electrochemical properties. *Electrochimica Acta*. 2006, **51**(10), 1974-1989. ISSN 00134686. Dostupné z: doi:10.1016/j.electacta.2005. 06. 027

Perovskite Single Crystals for Energy Conversion of Solar Radiation

Stevan Gavranović[1], Jan Pospíšil[2], Vítězslav Novák[3], Petr Vanýsek[4]

[1] Department of Physical and Applied Chemistry, Faculty of Chemistry, Brno University of Technology

Purkyňova 464/118, Brno, Czech Republic
xcgavranovic@vutbr.cz

[2] Material Research Centre, Faculty of Chemistry, Brno University of Technology

[3] Department of Electrical and Electronic Technology, Faculty of Electrical Engineering and Communication, Brno University of Technology

[4] Department of Electrical and Electronic Technology, Faculty of Electrical Engineering and Communication, Brno University of Technology

Modern optoelectronic devices (solar cells, photodetectors, LED) are highly dependent on silicon manufacturing processes, which include significant energy consumption (up to 1 000 kWh/kg-Si) and several toxic, flammable and explosive chemicals (e.g. lead, brominated flame retardants, cadmium and chromium) [1].

Most of energy required for pure silicon production is generated from coal-fired plants in China. Environmental effects of such production are still unknown. Therefore, researchers switch focus from silicon-based optoelectronic towards more environmentally friendly and cheaper materials, one of which comes in form of organic-inorganic hybrid perovskites (OIHP). OIHP are solution-processable materials with intriguing optoelectronic properties: tunable bandgaps, large optical absorption coefficient, high electron and hole mobility, long carrier diffusion length and lifetime, low exciton binding energy [2].

These properties enable them to become the heart of various optoelectronic devices such as solar cells, photodetectors and light-emitting diodes. Low energetic demands of perovskite production and wide spectrum of possible applications put them on the hotspot of ever-evolving field of semiconductor physics. Perovskite solar cells are the best example of progress in this field. Their efficiency has been enhanced to over 25.6 % in just a decade, which has surpassed polycrystalline silicon solar cells and is comparable to the monocrystalline silicon solar cells [3].

Perovskites are studied in various dimensions: quantum dots (0D) as promising light emitting material, polycrystalline thin films (2D) as an active layer of perovskite solar cells, and single crystals (3D) as an active layer in both solar cells and photodetectors [4].

Previous studies point out that monocrystalline perovskites show better intrinsic properties than its polycrystalline counterpart. In particular, voids and defect present in polycrystalline materials lead to fast degradation and loss of their optoelectronic properties. In comparison, the monocrystalline perovskites (single crystals) have less defects and are therefore characterized with higher electron and hole mobility, longer carrier diffusion length, higher stability toward ambient erosion, high temperature and moisture [5]. Even though very promising materials, their commercialization is still hindered by the two major obstacles: poor stability compared to silicon semiconductors and presence of lead in their structure. Theoretical part of our work deals with the properties and frequently used synthetic routes of $MAPbX_3$-based perovskite single crystals (X= Cl, Br or I). Possible future applications and problems which might slow down their commercialization are also discussed. Experimental part of our work describes $MAPbBr_3$ synthesis via inverse temperature crystallization (ITC) method, structural and optical properties of as-prepared single crystals and electrical characterization of Au/$MAPbBr_3$/Au light-sensitive assembly. Its parameters (responsivity, external quantum efficiency and specific detectivity) are calculated based on the spectral and switching (on/off) current responses. The material is further discussed as possible active component for photovoltaic panels and photodetectors.

References

[1] Dubey, S., Jadhav, N. Y., & Zakirova, B. (2013). Socio-Economic and Environmental Impacts of Silicon Based Photovoltaic (PV) Technologies. Energy Procedia, 33, 322-334. https://doi.org/10.1016/j.egypro.2013. 05. 073

[2] Rong, S. -S., Faheem, M. B., & Li, Y. -B. (2021). Perovskite single crystals: Synthesis, properties, and applications. Journal of Electronic Science and Technology, 19(2). https://doi.org/10.1016/j.jnlest.2021.100081

[3] Jeong, J., Kim, M., Seo, J., Lu, H., Ahlawat, P., Mishra, A., Yang, Y., Hope, M. A., Eickemeyer, F. T., Kim, M., Yoon, Y. J., Choi, I. W., Darwich, B. P., Choi, S. J., Jo, Y., Lee, J. H., Walker, B., Zakeeruddin, S. M., Emsley, L., et al. (2021). Pseudo-halide anion engineering for α-FAPbI3 perovskite solar cells. Nature, 592(7854), 381-385. https://doi.org/10.1038/s41586-021-03406-5

[4] González-Carrero, S., Galian, R. E., & Pérez-Prieto, J. (2015). Organometal Halide Perovskites: Bulk Low-Dimension Materials and Nanoparticles. Particle & Particle Systems Characterization, 32(7), 709-720. https://doi.org/10.1002/ppsc.201400214

[5] Li, J., Duan, J., Yang, X., Duan, Y., Yang, P., & Tang, Q. (2021). Review on recent progress of lead-free halide perovskites in optoelectronic applications. Nano Energy, 80.

Acknowledgement
I would like to thank my fellow colleagues that help me write my first conference paper. Special thanks goes to professor Oldrich Zmeskal and doctor Jan Pospisil.

Assessment of Degradation of Alkali--Activated Blast Furnace Slag Progress Using the Mercury Intrusion Porosimetry

Jan Hajzler[1], Petr Hrubý[1], Vlastimil Bílek[1]
a Libor Topolář[2]

[1] Brno University of Technology, Faculty of Chemistry, Institute of materials science

xchajzlerj@fch.vut.cz

[2] Brno University of Technology, Faculty of Civil Engineering

Alkali-activated systems (AAS) represent a low-carbon inorganic binder as an alternative to Ordinary Portland cement. The main benefits of AAS are the lower carbon foot-print and economic demands along with the superior durability in aggressive environments contrary to the OPC. The techniques like the determination of compressive and flexural strength are usually used for characterization of degradation processes since their realization is accompanied by the deterioration of these properties. The phenolphthalein technique or advanced instrumental techniques (SEM, XRD) can be used as well. This paper study the possibility of utilization of the mercury Intrusion porosimetry (MIP) to characterize the degradation of alkali-activated blast furnace slag. The degradation processes are dependent on the porosity or permeability of the material, as the penetration of the aggressive media into the internal structure is a key for the reaction to take place. The MIP is a suitable method for the characterization of material porosity, thus it can indicate which material will be more susceptible to degradation than the others. Moreover, it can characterize the chan-

ges taking place since the reactions like the decalcification are associated by the increase of the total porosity. Various alkaline activators (sodium water glass, sodium hydroxide, sodium carbonate) were used for alkali-activation of blast furnace slag in the same activator dosage (6 % Na_2O by the slag weight). A binder based on common cement (CEM III) was also prepared for comparison. Water to binder ratio was kept the same (w/b = 0.45). After the initial 28 days of hydration in water the testing samples (mortars with 3 : 1 sand : binder ratio) were immersed in various aggressive environments (CH_3COOH, $MgSO_4$, Na_2SO_4, NaCl, NH_4NO_3 and water for 84 days). Then the changes in porosity were characterized with the dependence on the time of degradation. It was found out that immersion in solutions of acetic acid (pH = 3) and ammonium nitrate (6M) had the most significant effect to both total porosity and the pore size distribution. Immersion in other environments did not cause any relevant changes.

Acknowledgement

This work was supported by specific research FCH-S-21-7553 and with the financial support by the project: GA19-04703S „The use of non-destructive methods for testing of the condition of degraded alkali-activated concrete“, with financial support from the Czech science foundation.

Hot Humid Air Cooling by Shell and Tube Heat Exchangers

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

[1] Brno University of Technology, Faculty of Chemistry, Institute of Materials Chemistry

Purkyňova 464/118, 612 00 Brno, Czech Republic
Petr.Horvat@vut.cz

[2] Brno University of Technology, Faculty of Mechanical Engineering, Heat transfer and fluid flow laboratory

Technická 2896/2, 616 69 Brno, Czech Republic

[3] Brno University of Technology, Faculty of Chemistry, Institute of Chemistry and Technology of Environmental Protection

Purkyňova 464/118, 612 00 Brno, Czech Republic

The processes of cooling gasses by shell and tube heat exchangers for subsequent application in processes of removal of gaseous air contaminants via liquid absorber is the major topic of this work. The aim of the work is to verify both the theoretical computational relations and the theoretical convenience of silicon carbide as a better heat transfer surface material compared with traditional borosilicate glass material characterized by two orders of magnitude worse thermal conductivity. The theoretical computational model using the j factor, the correction factors for the baffles, and the correction for air humidity condensation have been used.

Heat transfer on semi-operating shell and tube heat exchangers with glass or carbide heat exchange surface and baffles is exami-

ned by cooling the air by 50% propylene glycol in tubes having an inlet temperature just above 0 °C. Unfortunately, the coolant inlet temperature cannot be precisely regulated. Coolant flow can be regulated in many steps (max 24 m^3/h), but only laminar flow rates are available. Three-way flow of coolant is used. Air flow can be regulated by frequency changer (max 280 kg/h). Air could be heated up to 90 °C and the humidity of air could be increased by water stream with intensity up to 2,7 kg/h.

In previous experiments, local air heat transfer coefficient was low due to low ventilator power, the potential of the exchanger was not used also because of low temperature, and low humidity. Contrary to the assumption, new experiments with higher inlet air temperature resulted in a higher value of the heat transfer coefficient. The outlet temperature was only slightly higher than when measured without heater. The increase in humidity has a barely measurable effect on the heat transfer from the dry air. The effect of coolant flow on transferred heat is almost negligible. The efficiency of exchangers is very high (91–94 % with carbide and 88–89 % with glass), at higher temperatures even higher (up to 98 % with carbide and 96 % with glass).

Experiments with higher local air heat transfer coefficient are planned. More powerful ventilator will be installed, and the air flow will increase as well as heat transfer coefficient. Although devices increasing the enthalpy of currents have been installed, the potential of the exchangers was still far from being exploited. So, the temperature will be measured directly in the exchanger and the heat exchange in the beginning of the exchanger will be verified. Then, cooling of air will be situated in front of the separation of gaseous impurities from gas into liquid using a scrubber, more effective at lower temperatures. Separation of some pollutants could also take place by condensation in the exchanger at very low temperatures, or high pressures.

Determination of heavy and platinum group metals in rains settling tanks near highway

Stanislav Ježek[1], Renata Komendová[2]

[1] Stanislav Ježek, Institute of Chemistry and Technology of Environmental Protection, Faculty of Chemistry, Brno University of Technology

Purkyňova 464/118, Brno 61200, CZ
xcjezek@fch.vut.cz

[2] Renata Komendová Institute of Chemistry and Technology of Environmental Protection, Faculty of Chemistry, Brno University of Technology

Purkyňova 464/118, Brno 61200, CZ

Rain settlement tanks which collect and capture rainwater from specified drainage section of a highway D1 (Czech Republic) and in case of an accident with a substance leak, serve to capture the relevant unwanted liquid. In the case of precipitation, the water flows out of it after settling by an overflow into the adjacent water recipient such as river, stream or lake.

Intensive automobile traffic in Czech Republic is the reason for the release platinum and palladium to the environment. These metals form active layer in the automobile catalysts but there is significant leakage into the surrounding atmosphere during their use. Were analyzed water and sludge from rain settlement tanks and soil matrix which is near to rain settlement tanks. In view of the simpler diagnostics and more precise determination of the content of platinum and palladium, it is shown that the soil matrix and sludge are more suitable for studies of metal contents. In the case of the water samples, the sensitivity of the

determination was lower [1].

As a sampling point were chosen based on provided coordinates from organization Transport research centrum in the Brno. Sampling points are placed nearby the dam Švihov lake with distance between points less than 10 km.

Platinum and palladium are moving to the environment due to using autocatalysts in cars. Platinum metals are immobilized on the surface of the catalyst, where they are exposed to changing chemical, physical, and redox conditions that result in wear of the catalysts. [2] This wear leads to a gradual release into the environment during car operation. The obtained results show that the highest accumulation of platinum, palladium and heavy metals occurs in the soil and sediments of the monitoring tanks. [3]

References

[1] KOMENDOVA, R. a S. JEZEK. The distribution of platinum in the environment in large cities: a model study from Brno, Czech Republic. International Journal of Environmental Science and Technology. 2019, 16(7), 3109-3116. DOI: 10.1007/s13762-018-1954-x. ISSN 1735-1472. Dostupné také z: http://link.springer.com/10.1007/s13762-018-1954-xMilata V., Omastova M.: J. Org. Chem. 100, 1203 (2018).

[2] Platinum: ENVIRONMENTAL HEALTH CRITERIA 125 [http://www.inchem.org/documents/ehc/ehc/ehc125.htm]. Geneva: World health organization, 1991 [cit. 2018-04-07]. ISBN 92-4-157125-X. ISSN 0250-863X. Dostupné z: http://www.who.int/ipcs/publications/ehc/ehc_numerical/en/

[3] VLASANKOVA, Renata a Lumir SOMMER. Preconcentration Of Platinum Group Metals For Their Determination In Environmental Samples. DOI: 10.1080/10408347.1999.11978292. ISBN 10.1080/10408347.1999.11978292. Dostupné také z: https://www.tandfonline.com/doi/full/10.1080/10408347.1999.11978292

Thanks

This work was supported within the project FCH-S-21-7398, Ministry of Education, Youth and Sports of the Czech Republic.

Modification of Polyvinyl Alcohol to Increase Resistance to Moisture in MDF Composites

Jan Kotrla[1], Jiří Másilko[1], František Šoukal[1]

[1] Brno University of Technology, Faculty of Chemistry, Institute of materials science

xckotrla@fch.vut.cz

A Macro defect free (MDF) composites are materials consisting of inorganic cement and organic polymer. These materials have extreme mechanical properties that far outperform other cementitious materials and can compete with both ceramic and metal materials. Their mechanical properties are given by the minimization of pores and macro defects in the material and at the same time by mechanical-chemical interactions between cement and polymer. However, it is the presence of the polymer phase that reduce the moisture resistance of MDF composites. The water molecules travel along the structure of the polymer chain to the internal structure of the MDF composite, where the polymer swells and the cement hydrates additionally. This creates internal stresses, secondary defects and loss of mechanical properties. This work aims to increase the resistance of MDF composites to moisture. This can be achieved by increasing the density of the polymer phase by crosslinking the polymer. Maleic anhydride was selected as the crosslinking agent and grafted onto the polyvinyl alcohol polymer chain (GOHSENOL KH-17) in various batches. The amount of grafted maleic anhydride was determined by UV-VIS spectrometry. The measured values were further verified by FTIR spectroscopy and XPS analysis, which confirmed the increasing amount of maleic anhydride in the polymer chain. The resistance of the prepared samples to moisture was analysed using rheology. When the polymeric films were prepared and left under the action of water for 24 hours. Subsequently, the viscosity of the aqueous medium was measured. The highest resistance to moisture was observed in the sample with the highest degree of grafted maleic anhydride. To determine the mechanical properties, test specimens containing aluminous cement, modified polyvinyl alcohol, water and glycerol were prepared by twin-roll mixer. Flexural tensile strength was measured after 7 days. Samples were stored in a dry environment, at 100% humidity and under water. Here, as expected, the highest strength was found for samples stored in a dry environment. The highest strengths (65 MPa) were achieved by test specimens prepared from polyvinyl alcohol grafted with 20% maleic anhydride. When stored in 100% humidity, the strengths decreased by a quarter and when stored in water decreased by almost two third.

Acknowledgement

This work was supported by specific research FCH-S-21-7553.

CHLORINATED PARAFFINS AS PRECURSORS OF CHLORINATED PROCESSING CONTAMINANTS IN REFINED OILS

Tomáš Kouřimský[1], Jakub Tomáško[1],
Vojtěch Hrbek[1], Jana Hajšlová[1]

[1] UCT Prague, Faculty of Food and Biochemical Technology,
Department of Food Analysis
and Nutrition

Technická 3 166 28 Prague 6
kourimst@vscht.cz

Ester bound 2- and 3-chloropropanediol (2- and 3-MCPD) with fatty acids represent one of the most important groups of processing contaminants, contained primarily in refined oils, fats and products thereof. In recent years, considerable efforts have been made to understand the mechanisms of their formation including identification of their precursors [1,2].

The International Agency for Research on Cancer (IARC) classifies free 3-MCPD as a potential human carcinogen (Group 2 B). Although most of the 3-MCPD present in foods occurs in ester (approximately 85% diester and 15% monoester) bound forms, free 3-MCPD has been shown to be effectively released *in vivo* by the activity of lipolytic enzymes in the gastrointestinal tract. On this basis, in 2016 the European Food Safety Authority (EFSA) established a tolerable daily intake of 2 µg/kg body weight for 3-MCPD and its fatty acid esters, expressed as 3-MCPD equivalent, and in 2020 new maximum levels for 3-MCPD and its esters in oil and fats have been established. The required toxicological data for the risk assessment of 2-MCPD are not yet available [1-3].

A critical factor for MCPD formation is a chlorine source. Previous studies have shown that, besides inorganic chlorine compounds, organochlorine compounds (present in crude oils and fats mostly as exogenous contaminants), which might decompose under elevated temperatures. However, their structure, origin and potential contribution to MCPD formation is not yet fully understood [3-5].

The aim of this study was therefore to evaluate the potential of one group of lipophilic environmental contaminants - chlorinated paraffins (CPs) - to contribute to this process. These compounds were shown to be possible contaminants in crude oils and fats [6,7] and, therefore, potentially acting as chlorine donors for MCPD formation during oil refining process. For this purpose, laboratory scale model systems representing crude vegetable oil contaminated with CPs were designed and subjected to heat treatment to simulate the deodorization process. Varying degrees of MCPD formation and CPs decomposition were observed in crude palm oil samples. Nevertheless, these results could not yet be replicated in triolein systems and this topic requires further investigation as it uncovers more complex issues with each step.

References

[1] Albuquerque T. G., Costa H. S., Silva M. A., Oliveira M. B. P. P., *Trends in Food Science & Technology* 105 (2019) 494 – 514.
[2] EFSA, *EFSA Journal* 14 (2016).
[3] Bognár E., Hellner G., Radnóti A., Somogyi L., Kemény Z., *Period. Polytech. Chem. Eng.* 64
(2020), 523-529.
[4] Yao Y., Cao R., Liu W., Zhou H., Li C., Wang S., *J. Agric. Food Chem.* 67 (2019), 2700-2708.
[5] Tivanello R., Capristo M., Vicente E., Ferrari R., Sampaio K., Arisseto A., *J. Food. Sci.* 85 (2020), 2255-2260.

[6] Gao W., Bai L., Ke R., Cui Y., Yang C., Wang, Y., Jiang G., *J. Agric. Food Chem* 68 (2020),
7601-7608

[7] Cao Y., Harad, K. H., Liu W. Y., Yan J. X., Zhao C., Niisoe T., Adachi A., Fujii Y., Nouda C., Takasuga T., Koizumi A., *Chemosphere* 138 (2015) 104-111.

Acknowledgement

This work was supported from the grant of Specific university research – A2_FPBT_2021_020

Cesium halide perovskite as a material for scintillator detectors

Matouš Kratochvíl[1], Tomáš Musálek[2], Miroslav Kolíbal[2], Martin Weiter[1]

[1] Brno University of Technology, Faculty of chemistry

Purkyňova 118, Brno 612 00, Czech Republic
Matous.Kratochvil@vutbr.cz

[2] Brno University of Technology, Faculty of Mechanical Engineering

Technická 2896/2, Brno 616 00, Czech Republic

The enormous research attention given to hybrid organic-inorganic perovskite materials, a result of the unprecedented increase in perovskite based solar cell efficiency, helped to uncover their additional properties such as luminescence. These properties together with the presence of heavy Pb atoms makes hybrid perovskites an interesting candidate materials for radiation detectors. Nevertheless, the research also uncovered some crucial limitations like the susceptibility to external influences (moisture, UV radiation). The conducted studies usually ascribed this to the organic cation in the perovskite structure [1]. This discovery led to an intensive search for inorganic cations which could be used instead of the organic one, for example cesium cation Cs^+. Cesium lead halide perovskites show excellent luminescent properties [2,3] and are interesting candidates for use as scintillators for high-energy radiation detection. Cs perovskites in form of nanocrystal were reported as scintillators for X-ray detection with results comparable or better than the currently commercially used materials [4].

In our work we study Cs perovskites as possible materials for scintillators for detection of electrons (i.e. in electron microscopy). The preparation of nanocrystals by straightforward reprecipitation method is shown as well as characterization of resulting nanocrystals and prepared thin films.

References

[1] G. Niu, X. Guoa, L. Wang, *J. Mater. Chem. A* 3 (2015) 8970-8980.
[2] L. Gao, Q. Yan, *Sol. RRL* 4 (2020) 1900210.
[3] L. Protesescu, S. Yakunin, M. I. Bodnarchuk, F. Krieg, R. Caputo, C. H. Hendon, R. Xi Yang, A. Walsh, M. V. Kovalenko, *Nano Lett.* 15, 6 (2015) 3692–3696.
[4] J. H. Heo, D. H. Shin, J. K. Park, D. H. Kim, S. J. Lee, S. H. Im, *Adv. Mater.* 30 (2018) 1801743.

Acknowledgement

Authors gratefully acknowledge financial support from BUT under projects No. FCH/FSI-J-21-7396 and FCH-S-21-7553.

Dual-focus fluorescence correlation spectroscopy in the study of hydrogel properties

Kateřina Marková[1], Miloslav Pekař[2]

[1] Fakulta chemická, Vysoké učení technické v Brně

Purkyňova 118, 61700 Brno
Katerina.Markova@vut.cz

[2] Fakulta chemická, Vysoké učení technické v Brně

This contribution describes dependency of nanoparticles diffusion in the agarose hydrogel on the hydrogel concentration. The description of Brownian motion, in this case diffusion coefficient, can be measured by many techniques. Main disadvantage is the need to have a large amount of sample. For fluorescence correlation spectroscopy (FCS) techniques, it is necessary to have only few microliters of nanomolar concentration of the sample, also the confocal volume allows measurement of pretty small amount of the sample.

Unlike the single-FCS method, calibration is not required in dualfocus each time the temperature changes. Based on the optimization of the method and previous measurements, a suitable procedure for measuring the agarose samples was chosen. All data obtained from dual-focus FCS were compared with data measured using single-focus FCS. It was found, nanoparticles in water had very similar diffusion coefficient value. Significant differences were have been seen even at the lowest hydrogel concentration. Some of the autocorrelation curves had different shape compared with autocorrelation curves obtain form single-focus FCS.

For this type of measurement was chosen fluorescent labeled silica nanoparticles of suitable size for the selected hydrogel concentration.

Device for ionic exchange explanation: Organic electrochemical transistor in a fluorescence study

Aneta Marková[1], Martin Weiter[1], Martin Vala[1]

[1] Faculty of Chemistry, Brno University of Technology
Purkyňova 464/118, 612 00 Brno
xcmarkovaa@fch.vut.cz

The organic electrochemical transistor (OECT) is currently, among other things, a sought-after and researched device for its possible application in the field of bioelectronic devices, energy-harvesting technologies, sensing, etc. This transistor is based on the mixed ionic/electronic conductivity of organic semiconductors. These are referred to as supercapacitors. The development of such new organic semiconductors has a key role in expanding the portfolio of applications and especially in adapting their properties to the requirements of individual applications.

The organic electrochemical transistor is based on the principle of doping the entire volume of organic semiconductor with ions from the electrolyte. The degree of this doping is expressed by the value of transconductance, its equation is given by the channel parameters (width W, thickness d, and length L), volumetric capacitance C^*, mobility of charge carriers μ, and the magnitude of the applied voltage ($V_G - V_{Th}$), equation 1.

$$g_{\mathrm{m}} = \frac{Wd}{L} \mu C^* (V_{\mathrm{Th}} - V_{\mathrm{G}}) \qquad (1)$$

And it is the volumetric capacitance and mobility of charge carriers that are two key material parameters when comparing organic semiconductors from the perspective of electronic applications, and especially when designing these materials for use in OECT-based sensors. The volumetric capacitance of an organic semiconductor together with the mobility of charge carriers are the only two parameters of transconductance that cannot be influenced simply by changing geometric parameters or experimental conditions and govern the transconductance. However, the knowledge and ability to compare these values, especially the volumetric capacitance values, of individual organic semiconductors among themselves provide one of the possible ways to increase the overall sensitivity of OECT.

Although this is a figure-of-merit parameter, and there are a large number of publications, direct experimental determination of volumetric capacitance and understanding of its origin is still insufficient and is based primarily on various assumptions and theoretical models. This work deals with the possibility of studying the ion exchange between PEDOT:PSS and its environment (electrolyte) using two independent measurements (electrical detection using OECT and fluorescence detection using an ion-selective fluorescence probe).

By combining these two methods we would like to contribute to the understanding of the ionic exchange of organic semiconductors and for the most used one, poly(3,4-ethylene dioxythiophene):poly(styrene sulphonate), determine the amount of exchanged ions, thus the volumetric capacitance. The OECT was modified to enable fluorescence measurement, and the potassium ions exchange could be electrically and optically detected. We demonstrate that the fluorescence intensity decreases when the applied gate voltage is increased which corresponds to the assumptions (when is applied gate voltage potassium ions interact within the layer of organic semiconductor and the amount of ions in the electrolyte is decrease). This implies that the volumetric capacitance can be calculated using these two methods when the one calibrate these methods.

Acknowledgement
This research was supported by the Faculty of Chemistry at BUT under Project no. FCH-S-21-7301.

Poly(3-hydroxybutyrate) chain extension in the solution using bi- and trifunctional additives

Veronika Melčová[1], **Radek Přikryl**[1]

[1] Brno University of Technology, Faculty of Chemistry, Institute of Materials Chemistry

Purkyňova 464/118, 612 00 Brno, Czech Republic
xcmelcova@fch.vutbr.cz

For those, who are working with it, thermal degradation of poly(-3-hydroxybutyrate) (PHB) is a well-known phenomenon. What is not very clear is how to overcome this. Upon heating to the temperatures between 170 and 200 °C, which are the typical processing temperatures for PHB, the degradation is manifested by the change in molecular weight and viscosity of the system. Random scission is carried out by cis-elimination mechanism, also called McLafferty rearrangement [1-3]. One of the formed sub-molecules has an unsaturated crotonate end group and the other has carboxylate end group, which is theoretically prone to chain extension reaction which should lead to improvement of the thermal and mechanical performance of this polymer [4].

In this work, four functional groups reactive towards carboxyl group were studied: isocyanate, carbodiimide, hydroxyl and epoxy. Bifunctional reagents: hexamethylene diisocyanate, carbodiimide Stabaxol LF, diethylene glycol, and diglycidyl ether bisphenol A and trifunctional reagents: poly(hexamethylene diisocyanate), glycerol and trimethylol-propane triglycidyl ether were used. For the reactions, PHB was firstly pre-degraded in a laboratory hot press to mimic the degradation state obtained during processing. 5 wt% solution of

PHB in chloroform was prepared and after adding the reagent, the solution was kept under reflux for 6 hours. The reagent was added in two amounts corresponding to 2-fold and 100-fold overdose.

The effect of reagent addition was studied indirectly via change in the solution viscosity and directly by the change of molecular weight and thermal properties of the polymer.

For almost all the samples with bifunctional additives the solution viscosity was increased. The highest effect was observed in the case of diethylene glycol (+13.3 % in the case of 100-fold overdose). In the case of trifunctional additives, there was only slight rise for glycerol and trimethylol-propane triglycidyl ether for 2-fold overdose.

Similarly, the influence on molecular weight measured by gel permeation chromatography was more apparent for bifunctional additives. All trifunctional additives, together with some of the bifunctional successfully increased the number average molecular weight. The increase in weight average molecular weight was observed mainly in the case of 100-fold overdose of hexamethylene diisocyanate and carbodiimide samples, suggesting their potential use for chain extension of PHB during processing.

References

[1] N. GRASSIE, E.J. MURRAY and P.A. HOLMES, Polym. Degrad. Stabil. 6(1) (1984).
[2] N. GRASSIE, E.J. MURRAY and P.A. HOLMES, Polym. Degrad. Stabil. 6(2) (1984).
[3] F.-D. KOPINKE, M. REMMLER, and K. MACKENZIE, Polym. Degrad. Stabil. 52 (1) (1996.)
[4] C. R. ARZA et al., J. Appl. Polym. Sci. 132(15). (2015).

Acknowledgement

This work was supported by Specific University Research at FCH BUT, project FCH-S-21-7553, Ministry of Education, Youth and Sports of the Czech Republic.

Direct Potable Water Reuse through Pressure-driven Membrane Technology

Marek Minich[1], Martina Repková[1], Peter Putz[2], Michaela Vašinová Galiová[1,3]

[1] Brno University of Technology, Institute of Chemistry and Technology of Environmental Protection

Purkyňova 464, 612 00 Brno, Czech Republic
Marek.Minich1@vut.cz

[2] ASIO TECH l.t.d

Kšírova 552/45, 619 00 Brno, Czech Republic

[3] BIC Brno

Purkyňova 125, 612 00 Brno, Czech Republic

Recent drought period from 2014 to 2018 in Czech Republic have raised concerns about serious consequences of climate change for water availability in this region [1]. Municipal wastewater reuse could be a reliable and sustainable solution in cities and regions facing negative effects of drought [2]. In 2019, more than 790 million cubic meters of wastewaters were treated, and then discharged into recipients in Czech Republic [3].

On the other hand, this treated wastewater could be potentially returned to the urban water cycle. Pressure-driven membrane technology has an important role in water reuse in several potable water reuse applications across the globe [4]. For the needs of this study, an already existing pilot-scale ultrafiltration and reverse osmosis membrane unit was used to produce drinking water from the municipal wastewater treatment plant effluent. Such a configuration encloses the full cycle of wastewater management form the source through distribution, collection and treatment to its reuse which fully corresponds to the principles of the circular economy [5].

There were 44 physical, chemical and microbiological parameters observed to assess the quality of the produced water but input water as well. None of the parameters exceeded limit values issued by the Decree 70/2018 Coll. which determines hygienic requirements for drinking water in Czech Republic.

However, the produced water cannot be considered as drinking water, mainly, because of its low mineralization. Before its potential application in practice, it is therefore necessary to choose an appropriate method of remineralization as well as to follow all the other legislative requirements for the drinking water.

References

[1] M. Mozny, M. Trnka, V. Vlach, A. Vizina, V. Potopova, P. Zahradnicek, P. Stepanek, L. Hajkova, L. Staponites, Z. Zalud, *Journal of Hydrology* 2020, 590, 125390

[2] C. Y. Tang, Z. Yang, H. Guo, J. J. Wen, L. D. Nghiem, E. Cornelissen, *Environ. Sci. Technol.* 2018, 52, 18, 10215–10223

[3] D. Pokorný, E. Fousová, P. Hubalová, *Zpráva o stavu vodního hospodářství České republiky v roce 2019*, Prague, Czechia, 2020, p. 77.

[4] J. Lahnsteiner, P. van Rensburg, J. Esterhuizen, *Journal of Water Reuse and Desalination*, 2018; 8, 1, 14–28.

[5] M. Sgroi, F. G.A. Vagliasindi, P. Roccaro, *Curr. Opin. Environ. Sci. Health,* 2018, 2, 20-25

Acknowledgement

This research study was carried out in cooperation with the company ASIO TECH l.t.d.

Preparation and characterization of highly hydrophobic coatings on magnesium alloy AZ91

Šomanová Pavlína

Fakulta chemická, Vysoké učení technické v Brně

Purkyňova 464, 612 00 Brno, Czech Republic
somanova.p@seznam.cz

Magnesium and its alloys have many interesting properties and thanks to them it can be used in many applications (transport industry, medicine etc.). Disadvantage of these materials is their high corrosion rate. For this reason, there is an effort to achieve high corrosion resistance through different modifications of magnesium and its alloys. In recent years the superhydrophobization of the surface seem to be an attractive solution for this question. This type surface modification minimalize contact between the surface and water.

In this diploma thesis the superhydrophobic surface was created on the magnesium alloy AZ91. The first step included pretreatment of AZ91 surface by etching in solution of $SnCl_2$ or $ZnCl_2$. Next step was superhydrophobization in the ethanolic solution of stearic acid.

The surface morphology and elemental analysis of the superhydrophobic coating were explored by use of scanning electron microscope (SEM) and energy dispersive X-ray spectroscopy (EDS). The adhesion properties of the coating on the AZ91 were analysed by means of scratching test. Contact and sliding angles were measured for superhydrophobic coatings. Electrochemical characterization of the coatings was determined using potentiodynamic polarization (PD) and electrochemical impedance spectroscopy (EIS). Finally, the analysis of composition and the functional groups was made using Fourier-transform infrared spectroscopy (FTIR) and the phase composition analysis was performed using X-ray diffraction (XRD).

The results show that the coatings prepared by etching did not lead to good corrosion properties, even though the value of contact angle was about 150°. The reduction of corrosion resistance could be caused by not obtaining required surface morphology or insufficient binding of stearic acid in the form of stearate to the sample surface.

Characterization and Optimization of Novel Polymer Composite PEDOT:DBSA for Bioelectronic Applications

Romana Malečková[1], Šárka Tumová[1], Lubomír Kubáč[2], Jiří Akrman[2], Vojtěch Enev[1], Lukáš Kalina[1], Eva Šafaříková[3, 4], Jan Víteček[3], Martin Vala[1], Martin Weiter[1]

[1] Faculty of Chemistry, Brno University of Technology

Purkyňova 464/118, 612 00 Brno, Czech Republic
Romana.Maleckova@vut.cz

[2] Centre for Organic Chemistry

Rybitví 296, 533 54 Rybitví, Czech Republic

[3] Institute of Biophysics of the Czech Academy of Sciences

Královopolská 135, 612 65 Brno, Czech Republic

[4] Department of Experimental Biology, Faculty of Science, Masaryk University, University Campus Bohunice

Kamenice 5, 625 00 Brno, Czech Republic

Organic conducting materials represent a very promising alternative to traditionally used inorganic materials, especially in the fields of medicine and personalized treatment. Their unique properties give rise to many interesting next generation bioelectronic devices for various applications. PEDOT (poly(3,4-ethylenedioxythiophene)) doped with PSS (poly(styrenesulfonate)) is an organic polymer, which currently plays a main role in such applications, mainly because of its good processability and thermal and electrical stability. Nevertheless, recent research has shown minor cytotoxicity of the material attributed to the PSS moiety, whose sulfonate groups restrict cell adhesion. Therefore, the aim of this work was to introduce new conducting materials based on PEDOT, with improved properties compared with PEDOT:PSS. For this purpose, PEDOT doped with DBSA was studied.

This material proved its potential for bioelectronics, since it showed electrical properties comparable with PEDOT:PSS and other commonly used materials. However, two other key parameters limit the use of any material for such applications, stability in aqueous media and biocompatibility. In this study, PEDOT:DBSA has shown better long-term stability than PEDOT:PSS, which was further improved by cross-link. Cross-link also led to enhanced attachment of the material to the substrate and complete resistance against dissolution. Furthermore, the positive effect of the DBSA dopant on the materials biocompatibility was proven using standard MTT assay. Cells grown on pristine and also cross-linked material have shown almost twice as high relative viability compared with PEDOT:PSS and other commonly used organic semiconductors. This indicates that PEDOT:DBSA exceeds the properties of PEDOT:PSS and has a great potential for use in bioelectronic devices.

Acknowledgement

This work was supported by the Czech Science Foundation, project No. REG 21-01057S and by the Faculty of chemistry BUT under project No. FCH-S-21-7553

Novel Highly Stable Conductive Polymer Composite PEDOT:DBSA for Bioelectronic Applications

**Šárka Tumová[1], Romana Malečková[1],
Lubomír Kubáč[2], Jiří Akrman[2], Vojtěch Enev[1],
Lukáš Kalina[1], Eva Šafaříková[3, 4], Jan Víteček[3],
Martin Vala[1], Martin Weiter[1]**

[1] Faculty of Chemistry, Brno University of Technology

Purkyňova 464/118, 612 00 Brno, Czech Republic
xctumovas@fch.vut.cz

[2] Centre for Organic Chemistry

Rybitví 296, 533 54 Rybitví, Czech Republic

[3] Institute of Biophysics of the Czech Academy of Sciences

Královopolská 135, 612 65 Brno, Czech Republic

[4] Department of Experimental Biology, Faculty of Science,
Masaryk University, University Campus Bohunice

Kamenice 5, 625 00 Brno, Czech Republic

Organic bioelectronics presents a potential revolution in medicine as it holds the promise of personalised treatment. Conducting polymers have emerged as an excellent tool for bioelectronic devices due to their unique properties. Among them, PEDOT:PSS (poly (3, 4-ethylenedioxythiophene) doped with poly(styrenesulfonate)) has become increasingly selected as a material of choice for various applications thanks to its superior properties, especially excellent solution processability, electrical conductivity or stability. However, as recent research has shown, there are still limiting disadvantages of this material, light cytotoxicity and inadequate biocompatibility. These problems are attributed mainly to the presence of PSS moiety, which restricts the proper contact between material surface and living cells. Thus, the aim of this work was to propose a novel material with enhanced properties compared to PEDOT:PSS. To reach this, PEDOT doped with DBSA molecule was studied. It was proved that dopant DBSA itself has a positive effect on the biocompatibility of the polymer. Furthermore, the modification of material by cross-link provided excellent long-term stability. However, for bioelectronic applications, appropriate electrical properties present another key factor of essential importance. The electrical conductivity of pristine PEDOT:DBSA is of the same order as that of PEDOT:PSS. Even OECT based on this material showed behaviour typical for a p-channel transistor working in the depletion mode, with μC^* value comparable to other commonly used materials. But its cross-link had a significantly negative impact on electrical properties. This drawback was overcome using sulphuric acid post-treatment. The OECT based on such post-treated cross--linked material showed μC^* value even higher than pristine polymer. This shows the potential of PEDOT:DBSA, modified or not, for bioelectronic applications.

Acknowledgement

The work was supported by the Czech Science Foundation, project No. REG 17-24707S.

SYNTHESIS OF NEW PARA-BIS(2-THIENYL)PHENYLENE DERIVATIVES AS MOLECULAR PHOTOSWITCHES CANDIDATES

Dominik Veselý[1], Ján Jančík[1], Jozef Krajčovič[1]

[1] Brno University of Technology, Faculty of Chemistry, Institute of Chemistry and Technology of Environmental protection

Purkyňova 464/118, 612 00 Brno, Czech Republic
xcveselyd@vutbr.cz

Light is a noninvasive exogenous stimulus with high spatiotemporal resolution and precise remote on demand regulation of wavelength and intensity. Moreover, it does not cause contamination of samples. Thanks to these abovementioned characteristics, light can be considered as ideal candidate for *in situ* chemical and biological manipulation; it can be for example used to control the activity of biomolecules inside living cells selectively and specifically [1]. Molecular photoswitches are promising to serve for the above purpose as they undergo a characteristic change of their chemical structure upon light irradiation and consecutive photon absorption causing change to their respected chemical, physical, electrical and optical properties. This unique character together with wide range of possibilities for structural modifications on molecular level enables design and synthesis of new advanced molecular photoswitches tuned for specific applications [2].

This work is focused on synthesis of new para-bis(2-thienyl)phenylene derivatives with dodecyl and adamantyl-ethyl side chains. The basic trimer was prepared by the means of Kumada and Stille cross-coupling reactions via both conventional and microwave-

-assisted way. Another important goal of the research was the incorporation of the carbonyl functional group into the structure of the prepared trimer. This procedure was optimized through several synthetic approaches in the form of nucleophilic aromatic substitutions and nucleophilic additions. The carbonyl compound is a perfect intermediate for preparation of series of new derivatives by the means of condensation reactions; in this study a condensation with selected group of amines – aniline, 1-naphthylamine and 2-aminobenzothiazole was chosen. The imine C=N double bond is presented in the structure of the final products, thanks to which they are able to undergo a reversible *trans* to *cis* photoisomerization upon irradiation with 365 nm light. With consecutive relaxation in the dark, this whole process can be repeated with no significant sign of photodegradation. With the respect to these characteristics, prepared molecules are promising candidates for the applications in the field of molecular photoswitches.

References

[1] S. Jia, W. Fong, B. Graham, B. J. Boyd, *Chemistry of Materials* 30 (2018) 2873.
[2] I. Tochitsky, M. A. Kienzler, E. Isacoff, R. H. Kramer, *Chemical Reviews* 118 (2018) 10748.

Acknowledgement

This work was supported by the Internal Brno University of Technology project No. FCH-S-21-7553.

Key words

Molecular photoswitches, photoisomerization, imines, condensation reactions, organic synthesis.

Hydrogels with Gradient Properties

Natalia Zinkovska[1], Jiří Smilek[1], Miloslav Pekar[1]

[1]Brno University of Technology, Faculty of Chemistry, Institute of Physical and Applied Chemistry

Purkyňova street 118, 612 00 Brno, Czech Republic
xczinkovska@fch.vut.cz

Hydrogels are widely implemented materials of current importance due to their tunable and well customized functionality, reversibility, flexibility and biocompatibility. Unfortunately, homogeneous hydrogels cannot always satisfy the sophisticated demands of material engineering. For this reason, recently, there is a growing necessity in developing the materials with gradient properties for different application fields such as water treatment, tissue engineering, pharmacy, cell biology etc. Particularly, the gradient hydrogel has a progressive change in structure and function [1], that enables not only to mimic complex and anisotropic structures and control targeted release of active molecules or cell interactions, but also leads to more precisely adjustable application properties (transport, mechanical, separation).

Gradient hydrogels can be generated via various methods, providing either sharp or continuous physical and chemical gradients. Nevertheless the range of existing preparation methods is not universal. Each method is suitable for specific materials, requires certain equipment and has its own advantages and shortcomings. It should be noted, that common techniques for soft-material characterization are designed to analyze homogeneous samples. Hence, in the case of gradients, they must be adapted not only to inhomogeneous structures, but also to the copresence of chemical components or physical properties that can differ in satisfying the requirements for the use of a specific analytical technique [2]. Therefore the aim of presented study is to optimize selected preparation methods and characterization techniques, intended for gradient materials, and to analyze the main factors affected the creation and spatial distribution of the final gradient.

References

[1] LIU, Xin, Shuai LIU, Rong YANG, Penghui WANG, Wenjie ZHANG, Xiaoyan TAN, Yanhan REN a Bo CHI. Gradient chondroitin sulfate/poly (γ-glutamic acid) hydrogels inducing differentiation of stem cells for cartilage tissue engineering. *Carbohydrate Polymers*. **2021**, 270.

[2] SARDELLI, L, DP PACHECO, L ZORZETTO, C RINOLDI, W ŚWIĘSZKOWSKI a P PETRINI. Engineering biological gradients. *Journal of Applied Biomaterials & Functional Materials*. **2019**, 17(1), 1-15.

Synthon

teva

VYSOKÉ UČENÍ
TECHNICKÉ
V BRNĚ

FAKULTA
CHEMICKÁ