Selecting of a cytochrome P450<sub>cam</sub> SeSaM library with 3-chloroindole and endosulfan – Identification of mutants that dehalogenate 3-chloroindole

Cytochrome P450<sub>cam</sub> (a camphor hydroxylase) from the soil bacterium Pseudomonas putida shows potential importance in environmental applications such as the degradation of chlorinated organic pollutants. Seven P450<sub>cam</sub> mutants generated from Sequence Saturation Mutagenesis (SeSaM) and isolated by selection on minimal media with either 3-chloroindole or the insecticide endosulfan were studied for their ability to oxidize 3-chloroindole to isatin. The wild-type enzyme did not accept 3-chloroindole as a substrate. Mutant (E156G/V247F/V253G/F256S) had the highest maximal velocity in the conversion of 3-chloroindole to isatin, whereas mutants (T56A/N116H/D297N) and (G60S/Y75H) had highest $k_{cat}/K_M$ values. Six of the mutants had more than one mutation, and within this set, mutation of residues 297 and 179 was observed twice. Docking simulations were performed on models of the mutant enzymes; the wild-type did not accommodate 3-chloroindole in the active site, whereas all the mutants did. We propose two potential reaction pathways for dechlorination of 3-chloroindole. This article is part of a Special Issue entitled: Cytochrome P450 biodiversity and biotechnology, edited by Erika Plettner, Gianfranco Gilardi, Luet Wong, Vlada Urlacher, Jared Goldstone.
Latency and bit-error-rate evaluation for radio-over-ethernet in optical fiber front-haul networks

Nowadays several research projects are under progress to manage a soft migration toward the 5th generation networks. Radio over Ethernet (RoE) is one of recent topics that try to have a cost efficient and independent front-haul network. In this paper, we discuss the requirements of the 5G networks and analyze the conditions for the implementation of a RoE protocol. For this purpose we digitalize radio frames that are taken from BBU or RRH and create RoE basic frames considering all the requirements of protocol. We then encapsulate RoE basic frames into an Ethernet packet and finally experimentally evaluate this Ethernet packet as a case of study for RoE applications. The packet is transmitted through different fiber spans, measuring the BER and latency on each case. The system achieves BER values below the FEC limit and a manageable latency. These results serve as a guideline and proof of concept for applications on RoE, showing the viability of its implementation as part of the next generation of front-haul networks.

General information

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Organisations: Department of Photonics Engineering, Metro-Access and Short Range Systems, Networks Technology and Service Platforms, Electromagnetic Systems, Technical University of Denmark
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Scopus rating (2014): SJR 0.314 SNIP 0.839 CiteScore 1.39
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The UV filtering potential of drop-casted layers of frustules of three diatom species

Diatoms are in focus as biological materials for a range of photonic applications. Many of these applications would require embedding a multitude of diatoms in a matrix (e.g., paint, crème or lacquer); however, most studies on the photonic and spectral properties of diatoms frustules (silica walls) have been carried out on single cells. In this study, for the first time, we test the spectral properties of layers of frustules of three diatom species (Coscinodiscus granii, Thalassiosira punctifera and Thalassiosira pseudonana), with special focus on transmission and reflectance in the UV range. The transmittance efficiency in the UV A and B range was: T. pseudonana (56–59%) > C. granii (53–54%) > T. punctifera (18–21%) for the rinsed frustules. To investigate the underlying cause of these differences, we performed X-ray scattering analysis, measurement of layer thickness and microscopic determination of frustule nanostructures. We further tested dried intact cells in the same experimental setup. Based on the sedata we discuss the relative importance of crystal structure properties, nanostructure and quantity of material on the spectral properties of diatom layers. Characterization of the UV protection performance of layers of diatom frustules is of central relevance for their potential use as innovative bio-based UV filters.

General information
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Organisations: Department of Mechanical Engineering, Engineering Design and Product Development, National Institute of Aquatic Resources, Section for Oceans and Arctic, University of Copenhagen, International Iberian Nanotechnology Laboratory, Københavns Universitet
Authors: Su, Y. (Ekstern), Lenau, T. A. (Intern), Gundersen, E. (Ekstern), Kirkensgaard, J. J. K. (Ekstern), Maibohm, C. (Ekstern), Pinti, J. P. A. (Intern), Ellegaard, M. (Forskerdatabase)
Number of pages: 10
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.057 SNIP 1.684 CiteScore 5.3
Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 2.103 SNIP 1.544 CiteScore 4.75
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BFI (2013): BFI-level 1
A hamiltonian cycle in the square of a 2-connected graph in linear time

Fleischner's theorem says that the square of every 2-connected graph contains a Hamiltonian cycle. We present a proof resulting in an $O(|E|)$ algorithm for producing a Hamiltonian cycle in the square $G^2$ of a 2-connected graph $G = (V, E)$. The previous best was $O(|V|^2)$ by Lau in 1980.

More generally, we get an $O(|E|)$ algorithm for producing a Hamiltonian path between any two prescribed vertices, and we get an $O(|V|^2)$ algorithm for producing cycles $C_3, C_4, \ldots, C_{|V|}$ in $G^2$ of lengths 3, 4, \ldots, $|V|$, respectively.

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Dynamic bridge-finding in $\tilde{O}(\log^2 n)$ amortized time

We present a deterministic fully-dynamic data structure for maintaining information about the bridges in a graph. We support updates in $\tilde{O}(\log n)$ amortized time, and can find a bridge in the component of any given vertex, or a bridge separating any two given vertices, in $O(\log n \log \log n)$ worst case time. Our bounds match the current best for bounds for deterministic fully-dynamic connectivity up to $\log \log n$ factors. The previous best dynamic bridge finding was an $\tilde{O}(\log n)$ amortized time algorithm by Thorup [STOC2000], which was a bittrick-based improvement on the $O((\log \log n)^2)$ amortized time algorithm by Holm et al.[STOC98, JACM2001]. Our approach is based on a different and purely combinatorial improvement of the algorithm of Holm et al., which by itself gives a new combinatorial $\tilde{O}(\log n) \log \log n$ amortized time algorithm. Combining it with Thorup's bittrick, we get down to the claimed $\tilde{O}(\log n)$ amortized time algorithm. Essentially the same new trick can be applied to the biconnectivity data structure from [STOC98, JACM2001], improving the amortized update time to $\tilde{O}(\log n \log \log n)$. We also offer improvements in space. We describe a general trick which applies to both of our new algorithms, and to the old ones, to get down to linear space, where the previous best use $O(\log \log n)$ + $\log \log \log n$ space. Our result yields an improved running time for deciding whether a unique perfect matching exists in a static graph.
The bane of low-dimensionality clustering

In this paper, we give a conditional lower bound of $n^{\omega(k)}$ on running time for the classic $k$-median and $k$-means clustering objectives (where $n$ is the size of the input), even in low-dimensional Euclidean space of dimension four, assuming the Exponential Time Hypothesis (ETH). We also consider $k$-median (and $k$-means) with penalties where each point need not be assigned to a center, in which case it must pay a penalty, and extend our lower bound to at least three-dimensional Euclidean space. This stands in stark contrast to many other geometric problems such as the traveling salesman problem, or computing an independent set of unit spheres. While these problems benefit from the so-called (limited) blessing of dimensionality, as they can be solved in time $n^{O(k^{1-1/d})}$ or $2^{n^{1-1/d}}$ in $d$ dimensions, our work shows that widely-used clustering objectives have a lower bound of $n^{\omega(k)}$, even in dimension four. We complete the picture by considering the two-dimensional case: we show that there is no algorithm that solves the penalized version in time less than $n^{\omega(k)}$, and provide a matching upper bound of $n^{\omega(k)}$, even in dimension four. We complete the picture by considering the two-dimensional case: we show that there is no algorithm that solves the penalized version in time less than $[\text{Equation}]$, and provide a matching upper bound of $[\text{Equation}]$. The main tool we use to establish these lower bounds is the placement of points on the moment curve, which takes its inspiration from constructions of point sets yielding Delaunay complexes of high complexity.

Online bipartite matching with amortized $O(\log^2 n)$ replacements

In the online bipartite matching problem with replacements, all the vertices on one side of the bipartition are given, and the vertices on the other side arrive one by one with all their incident edges. The goal is to maintain a maximum matching
while minimizing the number of changes (replacements) to the matching. We show that the greedy algorithm that always takes the shortest augmenting path from the newly inserted vertex (denoted the SAP protocol) uses at most amortized $O(\log n)$ replacements per insertion, where $n$ is the total number of vertices inserted. This is the first analysis to achieve a polylogarithmic number of replacements for any replacement strategy, almost matching the $\Omega(n)$ lower bound. The previous best strategy known achieved amortized $\Omega(n)$ replacements [Bosek, Leniowski, Sankowski, Zych, FOCS 2014]. For the SAP protocol in particular, nothing better than then trivial $O(n)$ bound was known except in special cases. Our analysis immediately implies the same upper bound of $O(\log n)$ for the capacitated assignment problem, where each vertex on the static side of the bipartition is initialized with the capacity to serve a number of vertices. We also analyze the problem of minimizing the maximum server load. We show that if the final graph has maximum server load $L$, then the SAP protocol makes amortized $O(\min\{L, \log n\})$ reassignments for the capacitated assignment problem, where each vertex.

**General information**

State: Published  
Organisations: Department of Applied Mathematics and Computer Science, Algoritms and Logic, Technical University of Berlin, University of Copenhagen  
Authors: Bernstein, A. (Ekstern), Holm, J. (Ekstern), Rotenberg, E. (Intern)  
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10.1137/1.9781611975031.61  
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**Prototype of the novel CAMEA concept—A backend for neutron spectrometers**

**General information**

State: Published  
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Paul Scherrer Institut, University of Copenhagen, Ecole Polytechnique Federale de Lausanne (EPFL)  
Authors: Markó, M. (Ekstern), Groitl, F. (Ekstern), Birk, J. O. (Ekstern), Freeman, P. G. (Ekstern), Lefmann, K. (Ekstern), Christensen, N. B. (Intern), Niedermayer, C. (Ekstern), Jurányi, F. (Ekstern), Lass, J. (Ekstern), Hansen, A. (Ekstern), Rønnow, H. M. (Ekstern)  
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Web of Science (2016): Indexed yes
Relationship between PC index and magnetospheric field-aligned currents measured by Swarm satellites

Abstract The relationship between the magnetospheric field-aligned currents (FAC) monitored by the Swarm satellites and the magnetic activity PC index (which is a proxy of the solar wind energy incoming into the magnetosphere) is examined. It is shown that current intensities measured in the R1 and R2 FAC layers at the poleward and equatorward boundaries of the auroral oval are well correlated, the R2 currents being evidently secondary in relation to R1 currents and correlation in the dawn and dusk oval sectors being better than in the noon and night sectors. There is evident relationship between the PC
index and the intensity of field-aligned currents in the R1 dawn and dusk layers: increase of FAC intensity in the course of
substorm development is accompanied by increasing the PC index values. Correlation between PC and FAC intensities in
the R2 dawn and dusk layers is also observed, but it is much weaker. No correlation is observed between PC and field-
aligned currents in the midnight as well as in the noon sectors ahead of the substorm expansion phase. The results are
indicative of the R1 field-aligned currents as a driver of the polar cap magnetic activity (PC index) and currents in the R2
layer.

General information
State: Accepted/In press
Organisations: National Space Institute, Geomagnetism, Arctic and Antarctic Research Institute
Authors: Troshichev, O. (Ekstern), Sormakov, D. (Ekstern), Behlke, R. (Intern)
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BFI (2016): BFI-level 1
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.93 SNIP 0.943 CiteScore 1.48
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.966 SNIP 0.938 CiteScore 1.45
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.999 SNIP 1.146 CiteScore 1.73
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.165 SNIP 0.919 CiteScore 1.41
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.135 SNIP 1.061 CiteScore 1.64
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.519 SNIP 0.968
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.39 SNIP 1.163
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.22 SNIP 1.101
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.196 SNIP 1.106
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.232 SNIP 1.221
Scopus rating (2005): SJR 1.281 SNIP 1.197
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.162 SNIP 1.233
Scopus rating (2003): SJR 1.006 SNIP 1.262
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.822 SNIP 0.884
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.101 SNIP 0.843
Numerical modeling of the strand deposition flow in extrusion-based additive manufacturing

Abstract We propose a numerical model to simulate the extrusion of a strand of semi-molten material on a moving substrate, within the computation fluid dynamics paradigm. According to the literature, the deposition flow of the strands has an impact on the inter-layer bond formation in extrusion-based additive manufacturing, as well as the surface roughness of the fabricated part. Under the assumptions of an isothermal Newtonian fluid and a creeping laminar flow, the deposition flow is controlled by two parameters: the gap distance between the extrusion nozzle and the substrate, and the velocity ratio of the substrate to the average velocity of the flow inside the nozzle. The numerical simulation fully resolves the deposition flow and provides the cross-section of the printed strand. For the first time, we have quantified the effect of the gap distance and the velocity ratio on the size and the shape of the strand. The cross-section of the strand ranges from being almost cylindrical (for a fast printing and with a large gap) to a flat cuboid with rounded edges (for a slow printing and with a small gap), which substantially differs from the idealized cross-section typically assumed in the literature. Finally, we found that the printing force applied by the extruded material on the substrate has a negative linear relationship with the velocity ratio, for a constant gap.

General information
State: Published
Organisations: Department of Mechanical Engineering, Manufacturing Engineering
Authors: Comminal, R. (Intern), Serdeczny, M. P. (Intern), Pedersen, D. B. (Intern), Spangenberg, J. (Intern)
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Single-Phase Boost Inverter-Based Electric Vehicle Charger With Integrated Vehicle to Grid Reactive Power Compensation

Vehicle to grid (V2G) reactive power compensation using electric vehicle (EV) onboard chargers helps to ensure grid power quality by achieving unity power factor operation. However, the use of EVs for V2G reactive power compensation increases the second-order harmonic ripple current component at the DC-side of the charger. For single-phase, single-stage EV chargers, the ripple current component has to be supplied by the EV battery, unless a ripple compensation method is employed. Additionally, continuous usage of EV chargers for reactive power compensation, when the EV battery is not charging from the grid, exposes the EV battery to these undesirable ripple current components for a longer period and discharges the battery due to power conversion losses. This paper presents a way to provide V2G reactive power compensation through a boost inverter-based single stage EV charger and a DC-side capacitor without adversely affecting the EV battery. The operation of the boost inverter-based EV charger with second-order harmonic and switching frequency ripple current reduction, the dynamic behavior of the system, the transition between different operating modes, the DC-side capacitor voltage control above a minimum allowed voltage, and the DC-side capacitor sizing are extensively analyzed. The performance of the proposed system is verified using an experimental prototype, and presented results demonstrate the ability of the system to provide V2G reactive power compensation both with and without the EV battery.

General information
State: Published
Organisations: Department of Electrical Engineering, Center for Electric Power and Energy, Electric equipment technologies, University of New South Wales
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.498 SNIP 3.819 CiteScore 9.2
Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 2.299 SNIP 4.318 CiteScore 8.78
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.396 SNIP 4.427 CiteScore 8.41
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.945 SNIP 3.803 CiteScore 6.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.993 SNIP 3.359 CiteScore 7.12
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.796 SNIP 2.89
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.786 SNIP 2.726
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.538 SNIP 3.073
Web of Science (2008): Indexed yes
Scopus rating (2005): SJR 3.761 SNIP 3.411
Scopus rating (2004): SJR 2.931 SNIP 3.653
Scopus rating (2003): SJR 3.742 SNIP 3.056
Scopus rating (2002): SJR 3.953 SNIP 2.632
Scopus rating (2001): SJR 3.048 SNIP 1.904
Scopus rating (2000): SJR 0.664 SNIP 1.453
We describe magnetic fabric and depositional environments of aeolian (loess) deposits from Paks, Hungary, and develop a novel, complex conceptual sedimentation model based on grain size and low-field magnetic susceptibility anisotropy data. A plot of shape factor (magnetic fabric parameter) and dry deposition velocity estimated from grain-size reveals primary and secondary depositional processes during the sedimentation of loess. Primary ones are driven by gravity, with poorly oriented MF for fine grain materials, and by tangential stress, with flow-aligned or flow-transverse fabric for coarser grain sediments. The fabric developed by a primary process is called depositional magnetic fabric. Secondary processes develop in unconsolidated sediments, beginning right after deposition and terminating before the start of diagenesis. Under slow sedimentation conditions, deposited materials are likely to be exposed near the surface for longer periods. Therefore, relatively strong winds with a stable direction can alter the fabric of non-buried surficial sediments. As a result, grain orientations may change from scattered, non-flow oriented fabric to flow-oriented fabric. This type of fabric, developed by a secondary process, is called transformed magnetic fabric, and is characterized by relatively well-defined grain orientation, which allows us to estimate a dominant wind direction.

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Organisations: Center for Nuclear Technologies, Radiation Physics, Eötvös Loránd University, Kobe University
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Web of Science (2017): Indexed Yes
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Scopus rating (2016): CiteScore 2.44 SJR 1.113 SNIP 1.323
Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 0.98 SNIP 1.048 CiteScore 2.23
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Publication: Research - peer-review › Journal article – Annual report year: 2018
Complete Genome Sequence of Escherichia coli Strain WG5
Escherichia coli strain WG5 is a widely used host for phage detection, including somatic coliphages employed as standard ISO method 10705-1 (2000). Here, we present the complete genome sequence of a commercial E. coli WG5 strain.

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Organisations: Novo Nordisk Foundation Center for Biosustainability, Research Groups, Bacterial Synthetic Biology, Leibniz Institute for Natural Product Research and Infection Biology - Hans Knoll Institute (HKI), J, University of Barcelona
Authors: Imamovic, L. (Intern), Misiakou, M. (Intern), van der Helm, E. (Intern), Panagiotou, G. (Ekstern), Muniesa, M. (Ekstern), Sommer, M. O. A. (Intern)
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Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 0.199 SNIP 0.077
Scopus rating (2014): SJR 0.218 SNIP 0.089
ISI indexed (2013): ISI indexed no
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Synthesis of branched and linear 1,4-linked galactan oligosaccharides
We report the synthesis of linear and branched (1→4)-D-galactans. Four tetra- and one pentasaccharide were accessed by adopting a procedure of regioselective ring opening of a 4,6-O-naphthylidene protecting group followed by glycosylation using phenyl thioglycoside donors. The binding of the linear pentasaccharide with galectin-3 is also investigated by determination of a co-crystal structure. The binding of the (1→4)-linked galactan to Gal-3 highlights oligosaccharides of pectic galactan, which is abundant in the human diet, as putative Gal-3 ligands.

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Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen, SARomics Biostructure AB, Newcastle University
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Evaluation of ELISA and haemagglutination inhibition as screening tests in serosurveillance for H5/H7 avian influenza in commercial chicken flocks
Avian influenza virus (AIV) subtypes H5 and H7 can infect poultry causing low pathogenicity (LP) AI, but these LPAIVs may mutate to highly pathogenic AIV in chickens or turkeys causing high mortality, hence H5/H7 subtypes demand statutory intervention. Serological surveillance in the European Union provides evidence of H5/H7 AIV exposure in apparently healthy poultry. To identify the most sensitive screening method as the first step in an algorithm to provide evidence of H5/H7 AIV infection, the standard approach of H5/H7 antibody testing by haemagglutination inhibition (HI) was compared with an ELISA, which detects antibodies to all subtypes. Sera (n = 1055) from 74 commercial chicken flocks were tested by both methods. A Bayesian approach served to estimate diagnostic test sensitivities and specificities, without assuming any ‘gold standard’. Sensitivity and specificity of the ELISA was 97% and 99.8%, and for H5/H7 HI 43% and 99.8%, respectively, although H5/H7 HI sensitivity varied considerably between infected flocks. ELISA therefore provides superior sensitivity for the screening of chicken flocks as part of an algorithm, which subsequently utilises H5/H7 HI to identify infection by these two subtypes. With the calculated sensitivity and specificity, testing nine sera per flock is sufficient to detect a flock seroprevalence of 30% with 95% probability.
Methanation of CO\textsubscript{2} over Zeolite-Encapsulated Nickel Nanoparticles

Efficient methanation of CO\textsubscript{2} relies on the development of more selective and stable heterogeneous catalysts. Here we present a simple and effective method to encapsulate Ni nanoparticles in zeolite silicalite-1. In this method, the zeolite is modified by selective desilication, which creates intra-particle voids and mesopores that facilitate the formation of small and well-dispersed nanoparticles upon impregnation and reduction. TEM and XPS analysis confirm that a significant part of the Ni nanoparticles are situated inside the zeolite rather than on the outer surface. The encapsulation results in an increased metal dispersion and, consequently, a high catalytic activity for CO\textsubscript{2} methanation. With a gas hourly space velocity of 60000 ml/g catalyst h\textsuperscript{-1} and H\textsubscript{2}/CO\textsubscript{2}=4, the zeolite-encapsulated Ni nanoparticles result in 60\% conversion at 450°C, which corresponds to a site-time yield of around 304 mol CH\textsubscript{4}/mol Ni h\textsuperscript{-1}. The encapsulated Ni nanoparticles show no change in activity or selectivity after 50 h of operation, although post-catalysis characterisation reveals some particle migration.

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Isoenergetic modification of whey protein structure by denaturation and crosslinking using transglutaminase

Transglutaminase (TG) catalyzes formation of covalent bonds between lysine and glutamine side chains and has applications in manipulation of food structure. Physical properties of a whey protein mixture (SPC) denatured either at elevated pH or by heat-treatment and followed by TG catalyzed crosslinking, have been characterised using dynamic light scattering, size exclusion chromatography, fluorescence spectroscopy and atomic force microscopy. The degree of enzymatic crosslinking appeared higher for pH- than for heat-denatured SPC. The hydrophobic surface properties depended on the treatment, thus heating caused the largest exposure of the hydrophobic core of SPC proteins, which was decreased by crosslinking. The particle size of the treated SPC samples increased upon crosslinking by TG. Moreover, the particle morphology depended on the type of denaturing treatment, thus heat-treated SPC contained fibrillar structures, while pH-denatured SPC remained globular as documented by using atomic force microscopy. Finally, the in vitro digestability of the different SPC samples was assessed under simulated gastric and intestinal conditions. Notably heat-treatment was found to lower the gastric digestion rate and enzymatic crosslinking reduced both the gastric and the intestinal rate of digestion. These characteristics of the various SPC samples provide a useful basis for design of isoenergetic model foods applicable in animal and human studies on how food structure affects satiety.

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Tailored Electron Transfer Pathways in Aucore /Ptshell -Graphene Nanocatalysts for Fuel Cells

Aucore/Ptshell-graphene catalysts (G-Cys-Au@Pt) are prepared through chemical and surface chemical reactions. Au–Pt core–shell nanoparticles (Au@Pt NPs) covalently immobilized on graphene (G) are efficient electrocatalysts in low-temperature polymer electrolyte membrane fuel cells. The 9.5 ± 2 nm Au@Pt NPs with atomically thin Pt shells are attached on graphene via L-cysteine (Cys), which serves as linkers controlling NP loading and dispersion, enhancing the Au@Pt NP stability, and facilitating interfacial electron transfer. The increased activity of G-Cys-Au@Pt, compared to non-chemically immobilized G-Au@Pt and commercial platinum NPs catalyst (C–Pt), is a result of (1) the tailored electron transfer pathways of covalent bonds integrating Au@Pt NPs into the graphene framework, and (2) synergetic electronic effects of atomically thin Pt shells on Au cores. Enhanced electrocatalytic oxidation of formic acid, methanol, and ethanol is observed as higher specific currents and increased stability of G-Cys-Au@Pt compared to G-Au@Pt and C–Pt. Oxygen reduction on G-Cys-Au@Pt occurs at 25 mV lower potential and 43 A gPt−1 higher current (at 0.9 V vs reversible hydrogen electrode) than for C–Pt. Functional tests in direct fomic acid, methanol and ethanol fuel cells exhibit 95%, 53%, and 107% increased power densities for G-Cys-Au@Pt over C–Pt, respectively.

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Interaction between structurally different heteroexopolysaccharides and β-lactoglobulin studied by solution scattering and analytical ultracentrifugation

Despite a very large number of bacterial exopolysaccharides have been reported, detailed knowledge on their molecular structures and associative interactions with proteins is lacking. Small-angle X-ray scattering, dynamic light scattering and analytical ultracentrifugation (AUC) were used to characterize the interactions of six lactic acid bacterial heteroexopolysaccharides (HePS-1-HePS-6) with β-lactoglobulin (BLG). Compared to free HePSs, a large increase in the X-ray radius of gyration RG, maximum length L and hydrodynamic diameter dH of HePS-1-HePS-4 mixed with BLG revealed strong aggregation, the extent of which depended on the compact conformation and degree of branching of these HePSs. No significant effects were observed with HePS-5 and HePS-6. Turbidity and AUC analyses showed that both soluble and insoluble BLG-HePS complexes were formed. The findings provide new insights into the role of molecular structures in associative interactions between HePSs and BLG which has relevance for various industrial applications.

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On the contribution of reclaimed wastewater irrigation to the potential exposure of humans to antibiotics, antibiotic resistant bacteria and antibiotic resistance genes - NEREUS COST Action ES1403 position paper

Antibiotic resistance (AR) is becoming a worldwide threat due to the increasing occurrence of antibiotic-resistant pathogenic bacterial strains. There is a general consensus about the potential implications of the use of antibiotics in livestock on the onset of antibiotic resistant bacteria (ARB), mainly through meat consumption. However, the ever-increasing use of reclaimed wastewater (RWW) in agriculture may also contribute significantly to the non-accounted exposure to antibiotics, ARB, and antibiotic resistance genes (ARGs). This position paper aims at evaluating the current knowledge concerning the occurrence of antibiotics, ARBs, and ARGs in edible parts of different common crops irrigated with RWW. We will discuss which regulations on the use of RWW may contribute to the minimization of the prevalence of these contaminants in crops, and provide recommendations on how to minimize the impact of these practices.

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