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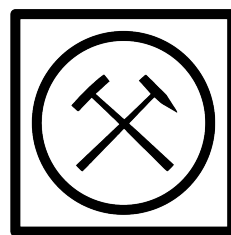Sustainability? - Your research - our world
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- Abstracts -

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List of oral presentations

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Oral Presentations

Pore scale modelling of multiphase flow using COMSOL Multiphysics® for enhanced oil recovery (EOR) applications

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Abstract

Understanding fluid flow phenomena in porous media is a crucial issue in petroleum, chemical, and material engineering. In oil and gas reservoir engineering, fluid flow simulation in porous media is one of the most powerful tools to predict reservoir behavior in the future and the response of the reservoir to different production scenarios and enhanced oil recovery (EOR) schemes that may be planned after primary recovery of the oilfield.

Volume averaging method is always used to simulate different transport phenomena in porous media including oil and gas reservoirs. However, in the last decade, pore scale modelling started to gain more attention by most of porous media's research groups all over the world owing to exponential growing of computational power and the emerge of HPC.

In this short communication, the difference between classical description of porous media and pore scale approach will be addressed. Pore scale simulation approach using phase field model will be highlighted with a 2D model example. The initial results show efficient description of real physics but need to be extended to 3D, which is computationally expensive. Finally, the future role of pore scale modelling to solve the problems of the brown oilfields will be discussed.

This study is the first step toward understanding multiphase flow and heat transfer at pore scale in porous media. Further steps in this direction are being under investigation.

Disappointment due to positive online reviews?
The counterproductive effect of positive online reviews in decision making under uncertainty

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Abstract

In this paper the author develops a mathematical concept to describe "disappointment" within the framework of expected utility theory. Disappointment is viewed here to be the nonachievement of customer's prior expectation (prior utility). Information asymmetry enhances this disparity between expectation and the actual outcome. To reduce this effect, customers deal with information search before making a buying decision. One of the most important information sources in e-commerce is online review, which delivers a wide range of information in a fast and convenient way. This information will help consumers generate the prior utility of a product. Positive online reviews do not just tend to increase the willingness to pay, buying intention. At the same time, they also raise the bar of expectation. If the expectation is not exceeded by the actual performance, the disconfirmation (according to C/D Paradigm) will emerge. Negative disconfirmation yields disappointment at the end. This paper reveals the counterproductive influences of positive online reviews and gives insight into the decision making process under uncertainty and how online reviews affect subsequent consumer affective reaction after purchasing choice.

Keywords: post-choice evaluation, online word of mouth, disappointment, utility function

Blessed is he who expects nothing, for he shall never be disappointed.

Alexander Pope, 1688–1744

Online reviews grow in importance nowadays. Across a wide variety of researches, the authors pointed out the positive relationship between positive online reviews and sales (Zhu und Zhang 2010), willingness to pay (Parry und Kawakami 2015, S. 195), which means positive reviewed products will be sold more and consumers are willing to pay more for such products. What happens actually when consumers read such positive reviews? Do positive online reviews just bring advantages? Do online

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reviews still affect the consumer behavior after the purchasing process?

Positive online reviews increase not only the willingness to pay, but also the expectation (prior estimated utility, in short: prior utility). In the case that the posterior utility doesn't meet the prior utility, disappointment emerges (van Dijk und Zeelenberg 2002). Bell defines disappointment as "a psychological reaction to an outcome that does not match up against expectation" (Bell 1984). Referring to Frijda's definition, disappointment can be viewed as the "nonachievement of an expected outcome" (Frijda 1986). We can also find theoretical supports from assimilation-contrast attitude theory (Sherif und Taub 1958), confirmation/disconfirmation paradigm (Boulding et al. 1993) or appraisal theory (Scherer et al. 2001). Higher expectations may give rise to more disappointment when the outcomes are lower than expected (van Dijk und Zeelenberg 2002). On the other hand, if the posterior utility exceeds the prior utility, consumers will savor elation. Disappointment and elation are two psychological consequences regarding to the comparison of prior utility and posterior utility (Bell 1984) . Van Dijk and Zeelenberg argued that the emotion „disappointment" has two aspects: outcome-related disappointment (hereafter ORD) and person-related disappointment (hereafter PRD) (van Dijk und Zeelenberg 2002).

In most cases, the prior utility differs from the posterior utility due to information asymmetry. Therefore, consumers are exposed to decisions involving uncertainty every day. Online reviews can provide more information in a convenient way. Such information can help to reduce the purchase risk (Bolton et al. 2004; Chen et al. 2011; Clemons et al. 2006; Forsythe und Shi 2003; Pavlou und Gefen 2004) besides product information. Further, online reviews help consumers estimate the prior utility of a product before purchasing it.

To model this decision making process under uncertainty, various theories are developed, such as expected utility theory, subjective expected utility theory, also known as Bayerisian decision theory, regret theory, prospect theory. However, which of those aforementioned theories are appropriate for our problem? To model the prior and posterior utility of consumers, various utility functions (linear, logarithmic, power, exponential) have to be considered. Which of them characterizes consumer behavior better in our case?

One of the most important theories to model an individual's decision-making behavior is McClelland's trichotomy of needs with aspect to need for achievement, need for power and need for affiliation (McClelland 1961; McClelland 1979, 1962, 1970, 1975; McClelland et al. 1976; McClelland und Burnham 1976; McClelland und Winter 1971). They are involved to explain the motivation of certain behavior. In this paper we focus on one of them: need for affiliation, which contributes to interpersonal interactions more than other two. Researchers explain the negativity effect (consumers weight negative information more heavily than positive information) as a function of the individual's social environment (Zajonc 1968; Feldman 1966; Kanouse und Hanson, JR. 1972). Thus need for affiliation referring social ties is considered in this paper. We propose, from reading similar online reviews, people with different severities of need for affiliation will get various utilities.

The second determinant observed is self-efficacy which originates from social cognitive theory (Bandura et al. 1977) and it measures the perception of an individual's ability to perform a particular behavior. Past research has already shown that certain behavior pattern is influenced by intrapersonal determinant, individuals' self-efficacy (Rimal und Flora 1998). Related to computer-mediated communication, two main types were derived from self-efficacy: computer self-efficacy and internet self-efficacy (Hsu und Chiu 2004; Salanova et al. 2000; Torkzadeh et al. 2006; Gist et al. 1989). Our study will put the emphasis on internet self-efficacy. Internet self-efficacy can be defined as an individual's beliefs about his/her ability to competently use the internet. According to Torkzadeh et al., people with high self-efficacy are proactive and can work longer with computers than those with low self-efficacy (Torkzadeh et al. 2006). Furthermore, they can obtain more knowledge with their computers (Salanova et al. 2000). To measure the internet self-efficacy, we will use the scale improved

by Kim and Glassman (Kim und Glassman 2013). We propose, from reading similar online reviews, people with different severities of internet self-efficacy will get various utilities.

Considering the consumer heterogeneity, how do online reviews affect this estimated utility of consumers with interpersonal attributes (such as need for affiliation and internet efficacy) differently? Do the interpersonal determinants also reveal the risk types of the consumers? Are consumers with high internet efficacy less risk-averse than others? This kind of relation conduces to help us parametrize utility functions.

Comparing the disparity of prior and posterior utility, we can identify two different psychological outcomes: elation or disappointment of the current customer journey. Moreover, this will be noted as experience und experience is a crucial component of further expectation (Holbrook 1999). This dynamic system can be described as follows:
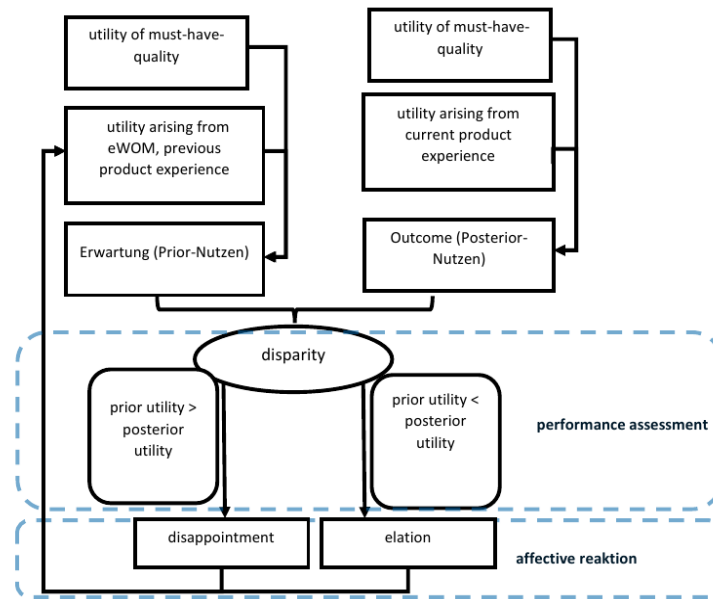

Figure 1: Based on C/D paradigm, Appraisal theory, Müller (Müller 2003)

This paper outlines the relationship between online reviews and psychological consequences of customer journey, especially the correlation between positive online reviews and disappointment. The author also shows the interaction between the interpersonal determinants and risk types. The focus on the discrepancy of the posterior and prior utility allows us a general predication without consideration of product categories, brand image and product involvement. Since the mathematical substitution eliminates automatically the constant factors, which just alter in a long period, in our case the utility of the must-have-quality, shortly: u_o. Using the utility function, we can model other components of prior and posterior utility as follows:

u_{eWOM} = utility from reading online reviews, u_{other} = utility from reading other information sources, $u_{current}$ = utility of arising from the actual product performance.

The disparity between posterior and prior utility can be illustrated therefore as $u_{current} - u_{eWOM} - u_{other}$.

Under the assumption that online review is the most important source of information, the utility function value of other source will fulfill $u_{other} \approx 0$ (for example, for movie market or new product market we have the equation, $u_{other} = 0$). Then the observed disparity can be written as:

$$Disparity = u_{current} - u_{eWOM} \ . \tag{1}$$

At the end, we will refine the results according to consumers with different interpersonal characteristics. The interaction between risk parameters and interpersonal determinants allows the expansion of the applicability of utility functions. The examination of the heterogeneity of individuals in terms of risk perception would help marketers target the appropriate messages.

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Sustainability in the Semiconductor Industry

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Abstract

This session shows the alternative methods for the etching of silicon nitride (Si_3N_4) on silicon wafers for sustainability in the semiconductor industry. Conventional processes operate with hydrofluoric acid or phosphoric acid. These are toxic and environmentally hazardous, contrary to the alternative etching agents. In this context a number of substances has been discovered that can etch the Si_3N_4 coatings. As representatives of this group one can name the following chemical compounds: Citric acid, thioglycolic acid glycine and glycolic acid. These substances lead to the chemical structure that the etchants must have in order to be corrosive to Si_3N_4. It must have an OH group or an analog in α and/or β position to a carboxylic acid.

In addition, first reaction mechanisms for the Silicon degeneration from the Silicon nitride surface postulated for this reaction (Figure 2). The group responsible for the degradation of silicon is the alcohol group or the analogue, represented as -XH. The Nitrogen degradation takes place by saturation with the aid of oxonium ions to ammonia and ammonium ions. According to Knotter and Denteneer (2001) [1] the preferred degradation is to ammonium ions.
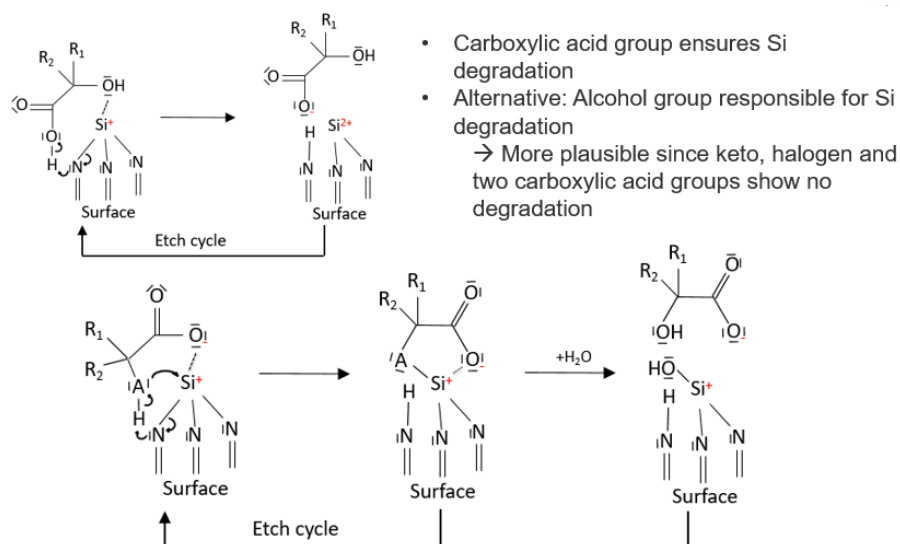

Figure 2: Postulated Si-Degradation Reactions.

Methods has been selected to characterize the discovered etchants more precisely. Therefore, ellip-

sometry and gravimetry are used as determining methods for measurement of the thin films. It was found that hydroxymalonic acid and lactic acid had the highest etch rates on a PECVD-Si_3N_4 coating at 4.7 $\mathrm{nm/h}$. On an LPCVD-Si_3N_4 coating, citric acid and hydroxymalonic acid exhibited the highest etch rates of up to 1.8 $\mathrm{nm/h}$.

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Synthesis of Mesoporous Resin Particles and Possible Application in Water Purification

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Abstract

Micro- and mesoporous polymers have received a significant increase in attention over the last two decades due to their unique properties such as high surface areas and scalable specific pore sizes, resulting in potential applications such as gas storage, advanced catalytic systems, semiconductor materials, and efficient adsorber materials [1]. Both persistent organic and inorganic water pollutants pose a risk for health and environment and therefore need to be eliminated from natural and industrial waters. Porous poly(melamine-co-formaldehyde) (PMF) combines the properties high porosity, functionality, and high chemical resistance due to the highly crosslinked polymer with a high percentage of nitrogen heteroatoms. The incorporation of this high amount of amino functionalities in the polymer provides an excellent potential adsorber material for both, cations and anions [2]. Hence, we investigated the synthesis of mesoporous PMF resin particles for the effective removal of heavy metal salts in water treatment [3, 4].

Mesoporous PMF particles with defined pore sizes were synthesized by an acid catalyzed dispersion polymerization of melamine and paraformaldehyde in water. Narrow-dispersed pore sizes were obtained by a hard templating method with silica nanoparticles. The impact of the acid, the amount of template and the concentration of formaldehyde and melamine in water on the particle formation will be presented.
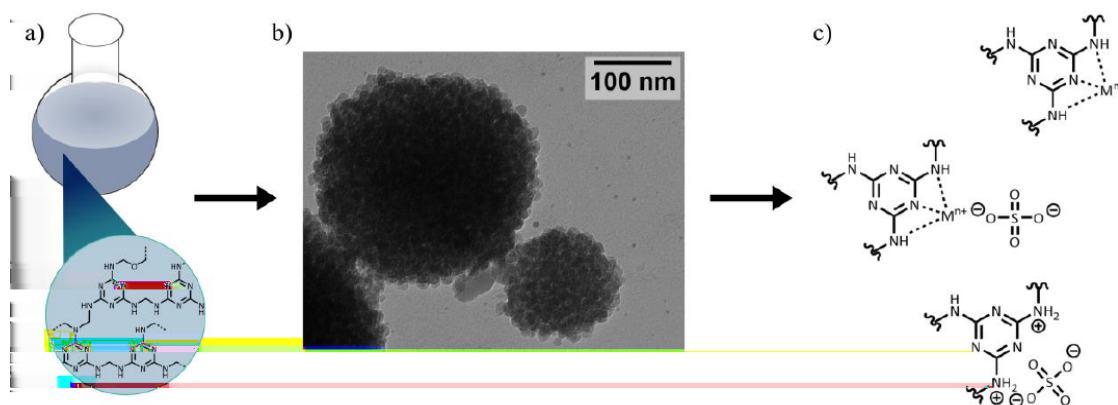
Figure 3: a) Polymerization of melamine, paraformaldehyde and silica nanoparticles in water, b) formed PMF particles, c) partial adsorption mechanism for heavy metal sulfates.

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The porous PMF particles were analyzed with microscopy (SEM and TEM), XRD and Nitrogen sorption (BET) experiments, supported by SAXS measurements. The composition was investigated by IR spectroscopy, TGA, and elemental analysis. The pure PMF particles were tested in individuaadsorption experiments with different heavy metal salts in batch experiments and the adsorption capacity was determined. PMF featured promising adsorption properties for oxyanions.

Acknowledgements

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Thermoelectric chalcogenides for waste heat recovery

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Abstract

Due to constant development of societies, global energy consumption is constantly increasing, e.g. by $38\,\%$ from 2000 to 2017 [1]. Thus, sustainability of technological processes and recovery of waste heat are leading research topics nowadays. One way to realize these goals involves thermoelectric (TE) generators. They are based on the TE materials that directly convert heat into electrical energy, thanks to Seebeck effect. Efficiency of such conversion is proportional to TE figure of merit $ZT = \alpha^2 \cdot \sigma \cdot \kappa^{-1} \cdot T$, which comprises three material's parameter: Seebeck coefficient α, electrical conductivity σ and thermal conductivity κ. Improvement of ZT requires simultaneous increase of α and σ and decrease of κ. Since all these parameters change in opposite way, optimization of the figure of merit is a great challenge. For instance, commercially produced TE modules are based on Bi_2Te_3 with $ZT \approx 1$ and reveal efficiency of only $5\,\%$ [2, 3]. Therefore, new materials with enhanced properties are required. In this context, two examples from our research on chalcogenides will be given: $Ag_{1-x}Sb_{1+x}Te_{2+x}$ and $In_{1-x}In_2S_4$ thiospinel. They are interesting for the study of TE properties due to extremely low thermal conductivity below $0.6\,\mathrm{W/m \cdot K}$ above room temperature. The former compound is well known as a component of highly efficient LAST (Pb-Ag-Sb-Te) and TAGS (Te-Ag-Ge-Sb) alloys and possess $ZT_{max} > 1$ above $600\,\mathrm{K}$ [4]. However, it reveals thermodynamic instability and gradually decomposes during operation. In-thiospinel possesses high Seebeck coefficient and is stable up to $760\,\mathrm{K}$, but its electrical conductivity still needs to be increased [5]. Challenges, results and difficulties of this study will be presented.

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CeMo$_2$B$_5$: a new type of arrangement of boron hexagonal rings

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Abstract

REMo$_2$B$_5$ (RE = Ce, Pr, Nd) and CeW$_2$B$_5$ have been synthesised by arc melting with further annealing at 1300 °C. CeMo$_2$B$_5$ is a new structure type crystallizing with $a = 11.0298(2)$ Å, $b = 3.12080(5)$ Å, $c = 9.9594(2)$ Å, SG *Pnma*, Z = 4. The structural arrangements reveal puckered [B6]-hexagonal ring, trigonal-prismatic- and empty polyhedron-slabs. The boron atoms form a two-dimensional network of corrugated ribbons, each composed of four linked [B6] rings infinitely extending along the *b*-axis. The small observed effective magnetic moment $\mu_{\mathrm{eff}} = 0.23(2)\,\mu_{\mathrm{B}}$ as well as theoretical DFT calculations confirm +4 oxidation state of Ce-ions. Electrical resistivity and Seebeck coefficient measurements together with the DFT calculations indicate CeMo$_2$B$_5$ to be a typical metallic system.

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A Review of the Socio-Environmental Impact Assessment of Artisanal and Small-scale Mining Operations in Western Ghana.

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Abstract

Highly proliferated and poorly regulated artisanal and small-scale mining (ASM) operations in Ghana have resulted in significant damages on the geo-environment. This paper presents an overview of the impacts of ASM in Western Ghana. Despite the ASM sector contributed about 30 % of the total gold production in 2016 and employs over 300,000 people in Ghana, their negative impacts are enormous. 312 communities within the western region of Ghana were observed to host over 7,400 individual mining operations. Of these, less than 5 % of them were observed to have been licensed to operate with the remaining been illegal operators. Their operations were ascertained to occur on productive farmlands, forests and protected areas, within communities as well as bodies of water. Even though data on current devastation levels are scanty, well over 60 % of forest and agriculture lands in the region are estimated to be lost to poor mining operations. These menace have not only remove vegetative covers but aided the extinction of endangered forest plants and animals as well as the loss of non-forest export products. Toxic chemical and metals have been released in concentrations higher than the EPA acceptable limits into the environment due to the bad mining cycles employed. Some water treatment facilities in host communities have been shut down due to high treatment cost and heavy siltation of water sources. An observed characteristic feature of ASM operators in Ghana are their highly aggressive and remarkably violent nature. Communities hosting such activities have high incident of violence and crime rates. Many farmers were observed to have lost their source of livelihoods directly by selling their lands or due to issues of insecurity. This condition has worsened the living standards of affected families leading to either rural-urban migration or becoming an accomplice of the miners for survival. Other reveal consequences were threat to food security, diseases outbreak, poor quality education, child labour issues as well as teenage pregnancies. This study established poor monitoring and policy enforcement by regulators, porous mining laws, high level of unemployment in the country as well as low political willingness of successive governments as the main driving force to these menace. No reclamation plans were observed to be instituted by these ASM operators leaving these lands in despair. Current ban on ASM operations in Ghana has received high level of resistance by the main ASM actors due to lack of a broad stakeholder consultation as well as the potential loss of sources of livelihoods. In furtherance, this study aims to develop a restoration mechanism for abandoned mined lands using local wastes and plants species as well as develop an integrated approach to managing ASM planning and closure systems in Ghana.

Microfluidic Synthesis of Inorganic Nanomaterials

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Abstract

Nanotechnology is the key technology of the 21th century, where new materials with specific and extraordinary properties, as for example core-shell structures, are designed to fullfill special and unique requirements in printed electronics and many other seminal applications.

Ongoing with new materials there is a need of new ways of synthesis, especially against the background of climate change and scarcity of resources. Microfluidic Synthesis of Nanomaterials offers a greener, smaller, better, faster and cheaper way of synthesizing organic, pharmaceutic, biological and inorganic nanomaterials with improved quality by simultaneously saving resources, improving yields, preventing side reactions and preventing a high chemical consumption. Additionally, because of dealing with low amounts of, for example explosive, chemicals in a closed system that can be handled in an automated, controlled and in-line supervised way, the safety standard of chemical synthesis can be improved enormously.

As the chemical reaction gets enclosed in a small reaction container in microsegmented flow regimes, the product quality raises drastically due to the fact, that every small reaction container experiences the same process history concerning reactant addition, mixing, heating, cooling and other impacts. Therefore, the products show a small particle size distribution and a high homogeneity in shape and composition, even for complex structures as nano-stars, -rods or -flowers. The synthesis is reproducible and adjustable to the desired product due to a variety of parameters and even multistep synthesis aren´t a problem anymore. This makes microfluidic synthesis of nanomaterials one of the most promising synthesis strategies at all.

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Natural microbial communities from Niger Delta facilitate anaerobic benzene mineralization under iron-reducing and methanogenic conditions

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Abstract

The Niger Delta region is one of the severely damaged ecosystems due to contamination with petroleum hydrocarbons that has not been sustainably managed. Anaerobic biodegradation is vital global carbon cycling mechanism where microbial communities degrade organic matters under a variety of redox conditions. Here, we present results for benzene mineralization of surface sediment sampled from Ogoni land (located at the western edge of the Niger Delta) under iron-reducing, sulfate-reducing and methanogenic conditions. Benzene was selected as model compound due to its toxicity and often observed persistence under anoxic conditions. We aim to evaluate the natural attenuation potential of Niger Delta sediments for anaerobic hydrocarbon degradation. Anaerobic mineralization of benzene was evaluated by analysis of produced $^{13}CO_2$ and $^{13}CH_4$ from ^{13}C-labelled benzene using gas chromatography-isotope ratio mass spectrometry (GC-IRMS). Putative anaerobic benzene-degrading key players were characterized by next-generation sequencing of the genes coding for 16S rRNA and methyl coenzyme M reductase A (mcrA). Additionally, single cells in iron-amended enrichment cultures were visualized by helium-ion microscopy. Benzene was slowly mineralized under iron-reducing and methanogenic conditions. Enrichment cultures amended with different iron sources mineralized benzene at different rates, but the highest rate was observed for one culture amended with iron (III) oxide. And cultures with iron nitrilotriacetic acid produced ^{13}C-labelled methane, indicating electron transfer from iron-reducers to methanogens. Syntrophic communities play key roles in which species cooperate to metabolize substrates in mutually beneficial manner. The predominant organisms of benzene-mineralizing enrichment cultures were phylotypes affiliated to Ignavibacteria and Proteobacteria (δ-Proteobacteria, α-Proteobacteria, γ-Proteobacteria), and methanogens of the genera Methanosarcina and Methanothrix, indicating that phylogenetically different organisms are involved in anaerobic benzene mineralization in the Niger Delta sediment samples. In conclusion, the results demonstrate a high natural attenuation potential of the investigated Niger Delta sediments for anaerobic hydrocarbon degradation especially under iron-reducing conditions.

Key words: Niger Delta; anaerobic degradation; benzene; natural attenuation; synthrophy

Electrical and thermal transport in high-quality polycrystalline and natural FeS$_2$

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Abstract

Synthetic polycrystalline and natural pyrite from the hydrothermal mine in Schönbrunn (Saxony, Germany) are stoichiometric FeS$_2$ compounds and stable (for thermoelectric applications) up to 600 K which was evidenced by combined thermal, chemical, spectroscopic and X-ray diffraction studies. Natural pyrite showed characteristics of a nondegenerate semiconductor and is suitable as a model system for investigation of thermoelectric performance. In the temperature range 50-600 K the electrical resistivity and Seebeck coefficient of polycrystalline samples became closer to Schönbrunn sample properties by longer annealing times under sulphur atmosphere. The large thermal conductivity in FeS$_2$ (40 W/m·K at 300 K) is exclusively due to lattice contribution. A well pronounced maximum in $\kappa(T)$ is observed only for natural pyrite at 75 K. This maximum becomes almost completely suppressed in the sintered samples (grain size $\leq$ 100 µm) due to additional scattering (i.e. point defect and/or grain boundaries) [1].

The thermoelectric performance of a highly-pure pyrite is not enough for the TE applications, however it seems to be a promising TE material due to the enhanced electrical transport properties observed in the studied natural samples.

Bibliography

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