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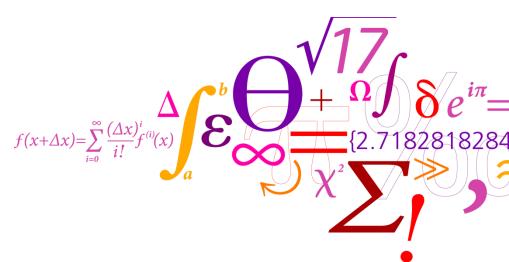
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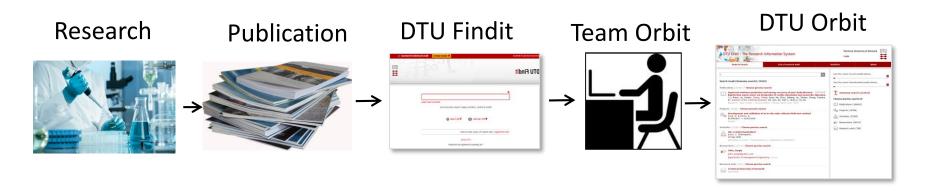
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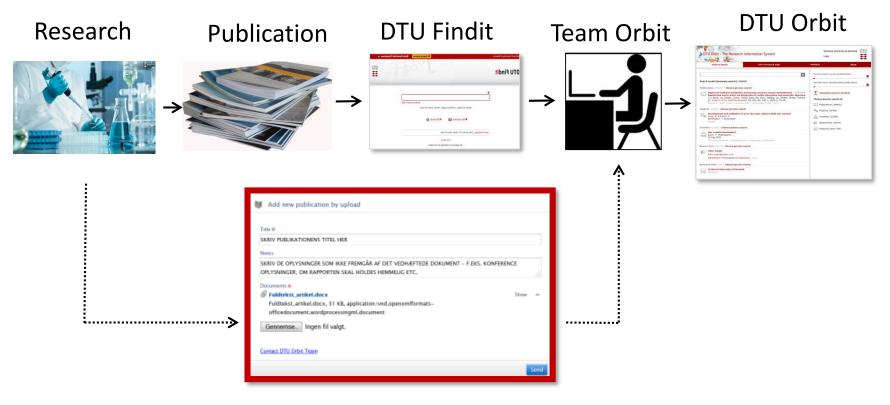


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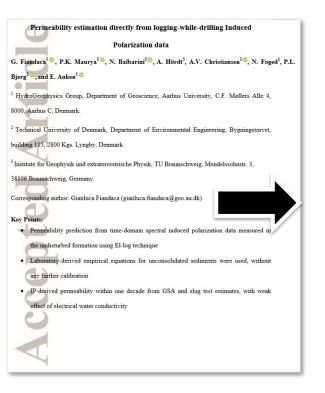


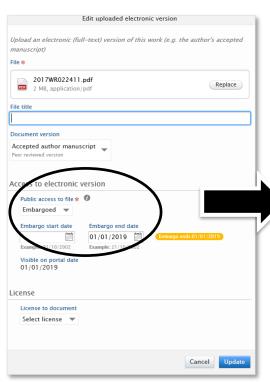
Central research registration at DTU - workflow



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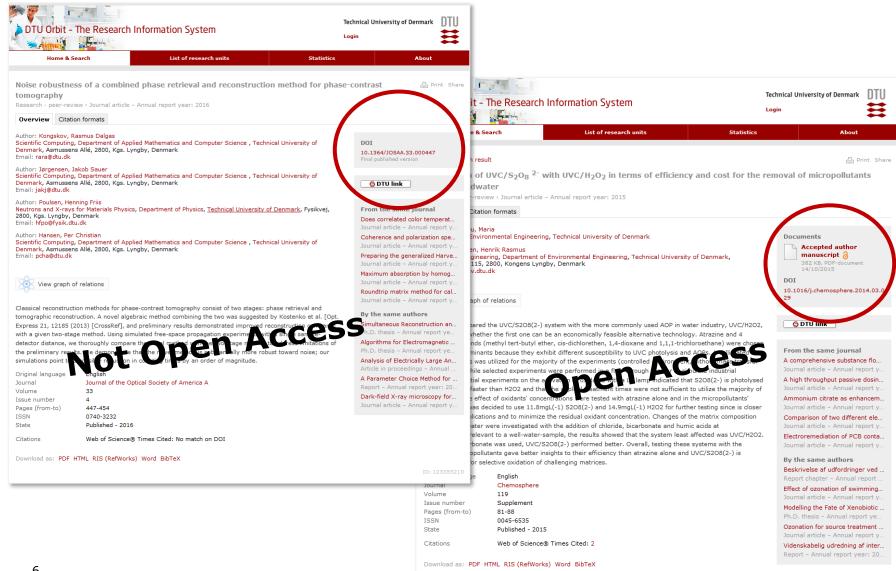
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- Accepted version
- Version 2
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- The peer-reviewed version
- Author Manuscript

The post-print has been peer-reviewed and accepted for publication. It includes the changes made as a result of the peer review process but lacks formal publisher layout.





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A Consistent Reaction Scheme for the Selective Catalytic Reduction of Nitrogen Oxides with Ammonia

Ton V. W. Janssens, Hanne Falsig, Lars F. Lundegaard, Peter N. R. Vennestrøm, Søren B. Rasmussen, Poul Georg Moses, Filippo Giordanino, Elisa Borfecchia, Kirill A. Lomachenko, Talo Lamberti, Silvia Bordiga,**,† Anita Godiksen,§ Susanne Mossin,**,§ and Pablo Beato*,†

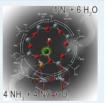
[†]Haldor Topsøe A/S, Nymøllevej 55, 2800 Kgs. Lyngby, Denmark

[‡]Department of Chemistry, INSTM Reference Center, University of Turin, Via Giuria 7, 10125 Torino, Italy

[¶]Southern Federal University, Zorge Street 5, 344090 Rostov-on-Don, Russia

Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Technical University of Denmark, Kemitorvet 207, 2800 Kgs. Lyngby, Denmark

ABSTRACT: For the first time, the standard and fast selective catalytic reduction (SCR) of NO by NH3 are described in a complete catalytic cycle that is able to produce the correct stoichiometry while allowing adsorption and desorption of stable molecules only. The standard SCR reaction is a coupling of the activation of NO by O2 with the fast SCR reaction, enabled by the release of NO2. According to the scheme, the SCR reaction can be divided into an oxidation of the catalyst by NO + O2 and a reduction by NO + NH3; these steps together constitute a complete catalytic cycle. Furthermore, both NO and NH3 are required in the reduction, and finally, oxidation by NO + O2 or NO2 leads to the same state of the catalyst. These points are shown experimentally for a Cu-CHA catalyst by combining in situ X-ray absorption spectroscopy (XAS), electron paramagnetic resonance (EPR), and Fourier transform infrared spectroscopy (FTIR). A consequence of the reaction scheme is that all intermediates in fast SCR are also part of the standard SCR 4 NH cycle. The activation energy calculated by density functional theory (DFT) indicates that the oxidation of an NO molecule by O2 to a bidentate nitrate ligand is rate-determining for



standard SCR. Finally, the role of a nitrate/nitrite equilibrium and the possible influence of Cu dimers and Brønsted sites are discussed, and an explanation is offered as to how a catalyst can be effective for SCR while being a poor catalyst for NO oxidation

KEYWORDS: SCR, fast SCR, rate-determining step, mechanism, Cu-CHA, NO oxidation, EPR, EXAFS, FTIR, XANES, DFT

1. INTRODUCTION

The selective catalytic reduction (SCR) of NO to N2 by ammonia (NH3-SCR) plays an important role in the abatement of NO, emissions in the exhausts of diesel engines and power plants. With environmental legislation becoming more stringent in many places in the world, this reaction is going to play an important role in the development of technologies to meet the emission requirements for exhaust gases. The commercially available catalysts for exhaust gas cleaning by NH3-SCR are based on vanadium oxide supported on titanium oxide, Feexchanged zeolites, or Cu-exchanged zeolites. The traditional zeolites applied in SCR are ZSM-5, and zeolite β. More recently, Cu-exchanged chabazites (CHA), in particular SSZ-13 and SAPO-34, have become more important because these materials are more stable under high temperature conditions. Other known Cu- or Fe-exchanged zeolites with SCR activity are SSZ-39,1 ferrierite, and mordenite.2,3

The composition and temperature of the exhaust gas from which the NO is to be removed depends on the source. In an automotive diesel engine, a typical exhaust gas contains up to a few hundred parts per million of NOz, 5-10% water vapor, 510% O2, hydrocarbons, CO, and CO2. Ammonia is usually introduced by decomposition of urea to a concentration level of typically 1.0-1.2 times the NO concentration; the slight excess of ammonia ensures an efficient removal of the NO. In a typical exhaust aftertreatment system, the hydrocarbons and CO are removed upstream from the SCR catalyst, and hence, the SCR catalyst is exposed to a mixture of NO, O2, H2O, and NH3 in an inert gas (N2 and CO2). The temperature at the SCR catalyst varies, and it is generally required that the SCR catalyst performs well in the temperature range 200-500 °C. This gas composition and temperature range define the general operation conditions for an SCR catalyst system.

The key reaction in the NH3-SCR is the formation of nitrogen from NO and NH3 according to the equation

$$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O$$
 (1)

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ACS Catalysis

A consistent reaction scheme for the selective 10 catalytic reduction of nitrogen oxides with 12 13 14

> Ton V. W. Janssens, Hanne Falsig, Lars F. Lundegaard, Peter N. R. Vennestrøm,† Søren B. Rasmussen,† Poul Georg Moses,† Filippo Giordanino,‡ Elisa Borfecchia, Kirill A. Lomachenko, T. Carlo Lamberti, J. Silvia Bordiga, J. Anita Godiksen,§ Susanne Mossin,*.§ and Pablo Beato*.†

ammonia

Haldor Topsøe A/S, Nymøllevej 55, 2800 Kgs. Lyngby, Denmark, Department of Chemistry, NIS Centre of Excellence and INSTM Reference Center, University of Turin, Via Giuria 7, 10125 Torino, Italy, Southern Federal University, Zorge Street 5, 344090 Rostov-on-Don, Russia, and Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Technical University of Denmark, Kemitorvet 207, 2800 Kgs. Lyngby, Denmark

E-mail: siliva.bordiga@unito.it; slmo@kemi.dtu.dk; pabb@topsoe.dk

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^{*}To whom correspondence should be addressed

[†]Haldor Topsøe

[‡]University of Turin

Southern Federal University Rostov-on-Don

[§]Technical University of Denmark



Interference Ascorbic Acid De

Hongyan Bi **, Ana C

⁵ International Iberian Nanotechnology ⁶ INESC Microsistemas e Nanotecnolo

> * Correspond Tel: +31

* Present address: CAPEC-PROCE

Abstract

A microfluidic sensor is devel drug food beverage matrices. The surfi modified by enzyme viz physisorption microfluidic channel, enzyme-catalyze products. The whole process is monito oxidase and L-ascorbic acid (AA) are feasibility of using the developed strate; matrices. A dietary supplement productrofluidic bio-sensor in real-sample sensor exhibits good reproducibility, s realize, depends on low investment in UV/vis spectrophotometer is required accurate, and can be potentially used fi background. It is promising to be widely

Keywords: microfluidic sensor; enz spectroscopy; ascorbic acid

Biofuels and Environmental Biotechnology

Biotec DOI 10

Linking hydrolysis performance to Trichoderma reesei

Linda Lehmann**¹, Nanna Petersen*², Christian I. Jørgensen*, Lisl S. Jørgensen* and Timothy Hobley*³.

*Center for Microbial Biotechnology, Department of Systems Biolo 2800 Kgs, Lyngby, Denmark

Department of Chemical and Biochemical Engineering, Technical Lyngby, Qenmark

Ñovozymes A/S, Krogshøjvej 38, 2880 Bagsværd, Denmark findustrial Biotechnology, Department of Chemical and Biological Technology, 412 98 Göteborg, Sweden

*Corresponding author

Email: Ile@novozymes.com

Present address: Novozymes A/S, Krogshøjvej 36, 2880 Bagsværd, Denmark
Prejsent address: Novo Nordisk A/S, Novo alle, 2880 Bagsværd, Denmark
Prejsent address: Division of Industrial Food Research, National Food Institute
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Experimental and in-silico investigation of population heterogeneity in continuous Sachharomyces cerevisiae scale-down fermentation in a novel two-compartment setup

Anna-Lena Heins 1,2 , Rita Lencastre Fernandes 2 , Krist V. Gernaey 2 and Anna Eliasson Lantz 1,2 !

Department of Systems Biology, Technical University of Denmark, 2800 Kongens Lyngby, Denmark

² Department of Chemical and Biochemical Engineering, Technical University of Denmark, 2800 Kongens Lyngby, Denmark

*These authors contributed equally to the work

⁶Corresponding author, email: <u>aela@kt.dtu.dk</u>, phone: +4545252851

Abstract

Background. In large-scale bioreactors, microbes often encounter fluctuating conditions of nutrient and oxygen supply, resulting in different microbial behavior at the different scales. The underlying reason being spatial heterogeneity, caused by limited mixing capabilities at production scale. Consequently, scale-up of processes is challenging and there is a need for laboratory-scale reactor setups that can mimic large-scale conditions to enhance the understanding of how fluctuating environmental conditions affect microbial physiology.

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A combination model with variable weight optimization for shortterm electrical load forecasting



Wei-Qin Li *.h.", Li Chang "

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ARTICLEINTO



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ABSTRACT

The present entry could letter a relicat combination forecasting model and achieves the accurate predistant of electrical load by considering the depresionary of the load series and the merconological factors. On this hars, the culture particle energy aprimitation algorithm is developed in improve the antenny of the Europea. The most is that by the particle mixation strongs, passenger adjustment unstray. depression on the Reess and the browings updating studing particles are assisted to map in local optimies, originally transming the computational speed and performance. Moreover, the data preprocessing technology hand so the ESSD is proposed to contact the tundent roles of the hand arrive and to theyeve the ratios of the land arrive and to theyeve the ratios of the tune of the probability distribution of relative errors. To assess the applicability and acrossing of the proposed model, is is compared with an culory optimization, griech: algorithm, constant annualing approach, exclose search algorithms, differential evaluation and artificial congernative acords. Receivs substantilly the armal data with the Shaunal province, China, alson higher securary and honor reliability of the proposed model

1. Introduction

The electrical load ferenanting plays an important rule in the economical and safe specialism of the modern power system. important decisions are made on account of the load forecasting, including the generating capacity, the relability analysis of the scheduling plan, the safety accounters and the maintenance plan. The load forecasting becomes more important with the rise of thee competition in the procer industry [1]. However, the had is affected by the weather, the builday and overpreted factors, etc [2,2], and than the half series have obvious variability and non-stationary. Here, the shoot-nern power had is increasingly difficult to firecast, but it is important for the system scheduling and the corning state equitoring. Therefore, it becomes imporative to develop the effective forecasting method with higher accessory and speed.

The data proper crosing is the key process of the load forecasting. and nightly includes noise reduction and the absormal data

* Companing artist School of Submitter and Information Engineering, Wast Makeusky of Trained up, War, 1988; Class.



processing. First, the random noise can reduce the reliability of prediction models and the position of the forecasting, Some forecasting methods samplesed with reported transferm can extract the series information at different sime scales and reduce the influence of eather, which have high accuracy, but are difficult to accurately select the superiet function and the decomposition scale \$4.55. Furthermore, the actual electrical local may contain the arenoutly data that seriously affects the formanting performance; and be caused by the smoot faults, power supply equipment full arm and other unimported events. Generally the amonally flara in descript according to the relative even between the forecasting data and the actual one. In traditional methods, the cumulative distribution of the rotative error is assumed to obey the specific distribution (note as a distribution, Carm distribution) [1] #1]. However, there is a deviation from the true probability distribution of rotative errors, and therefore reduce the reliability of the animaly detection.

In the short dress power lead forecasting (STUE), she forecasting techniques can be classified jobs: statistical models including the linear regression model (III), the time series method such as the autoregressive integrated moving average (ABSAN) model (101), the









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Danish National Strategy

The National Strategy is stating that by 2025 100 % of Danish peer-reviewed scientific articles JOU to or Danish Research institutions must be published Open Access. The implementation is to paulished open Access. The implementation is a take place through the green model. The use of the golden model is not excluded as long as it does not increase the expenses.

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Open Access figures* as of 12 May 2016	2015	2016	 2017	2022
The National Open Access Indicator**	20,59%	14,17%	80%	100%

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A) OPEN ACCESS: Artikler fra tidsskrifter uden postprint

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1. Publications

Analysis of Count on Publications

Туре	2017	2018
Contribution to journal - Journal article	19	24
Contribution to journal - Conference article	1	
Total	20	24

The above report is produced using the following setup

Limited by: Associated organisational unit = Department of Bio and Health Informatics; With internal affiliation; Current publication status > Status is one of E-pub ahead of print, Published, Accepted/In press; Calendar year(s) (1 Jan 2017 - 31 Dec 2018); Open Access status is not one of Open, Embargoed; Type is one of Journal article, Conference article, Review; Publication category is one of Research, Commissioned; Set Grouped on: Type; Submission year

2. Publications

Listing of Publications

Alvarez, B., Barra, C., Nielsen, M., & Andreatta, M. (2018). Computational Tools for the Identification and Interpretation of Sequence Motifs in Immunopeptidomes. *Proteomics*, [1700252]. DOI: 10.1002/pmic.201700252

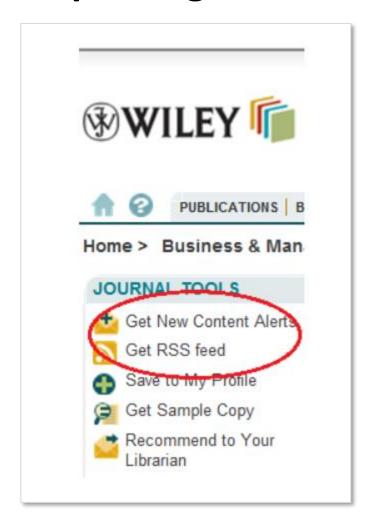
Andreatta, M., Trolle, T., Yan, Z., Greenbaum, J. A., Peters, B., & Nielsen, M. (2018). An automated benchmarking platform for MHC class II binding prediction methods. *Bioinformatics*, *34*(9), 1522-1528. DOI: 10.1093/bioinformatics/btx820

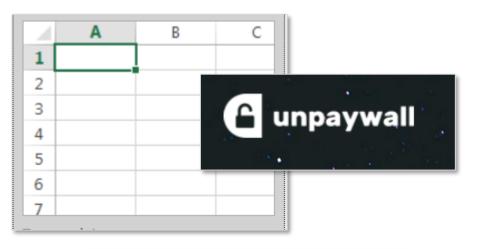
de Barros Damgaard, P., Martiniano, R., Kamm, J., Moreno-Mayar, J. V., Kroonen, G., Peyrot, M., ... Willerslev, E. (2018). The first horse herders and the impact of early Bronze Age steppe expansions into Asia. *Science*, [eaar7711]. DOI: 10.1126/science.aar7711

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Publications	
Scientific articles with referee in ISI-indexed journals	
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Books and contributions to books	
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Contributions to books and reports	
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Improving workflows





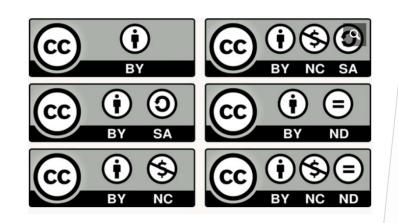


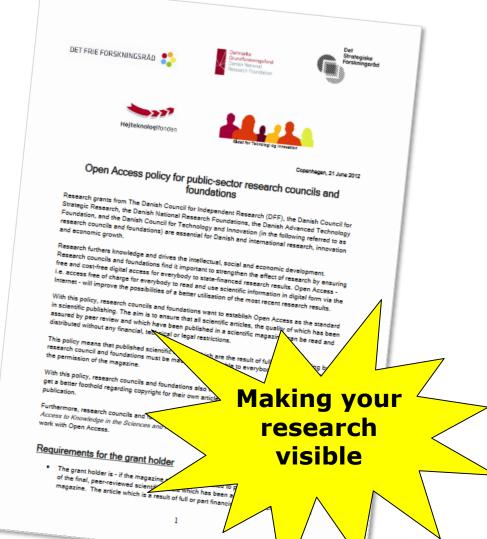




Enquiries, lectures, talks & courses



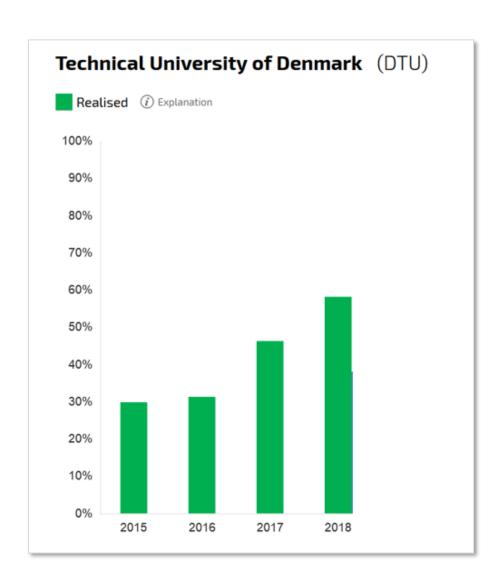




Still a long way to go but ...



- Long embargo periods
- Unclear publisher policies
- Submission templates
- Inconvenient IT infrastructure
- Etc. etc.





Questions?

