Open Access

DTU Library Services and Support

Maria Ravnkilde Christensen
Information consultant

DTU Library
Technical Information Center of Denmark

The Danish National Strategy

DTU Library’s Open Access services all relate to supporting the effort of DTU to comply with the Danish National Open Access Strategy

Service/support:

- Practical workflow

- Communication & outreach activities

Central research registration at DTU - workflow

Research

→

Publication

→

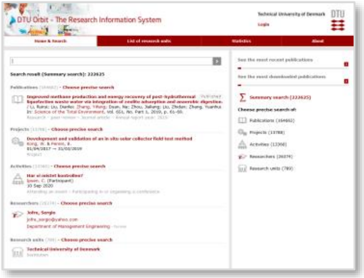
DTU Findit

→

Team Orbit

→

DTU Orbit



Central research registration at DTU - workflow

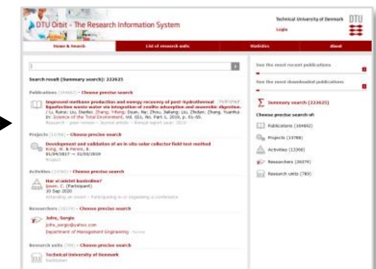
Research

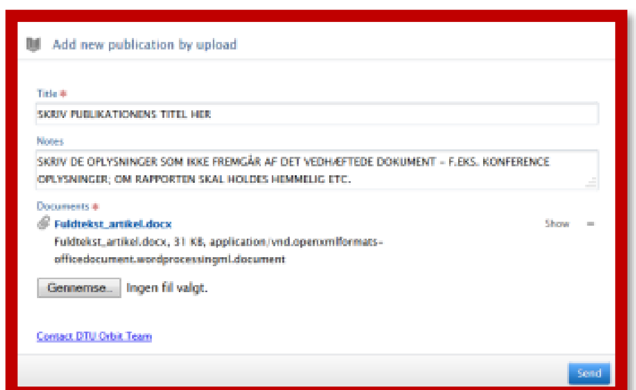
Publication

DTU Findit

Team Orbit

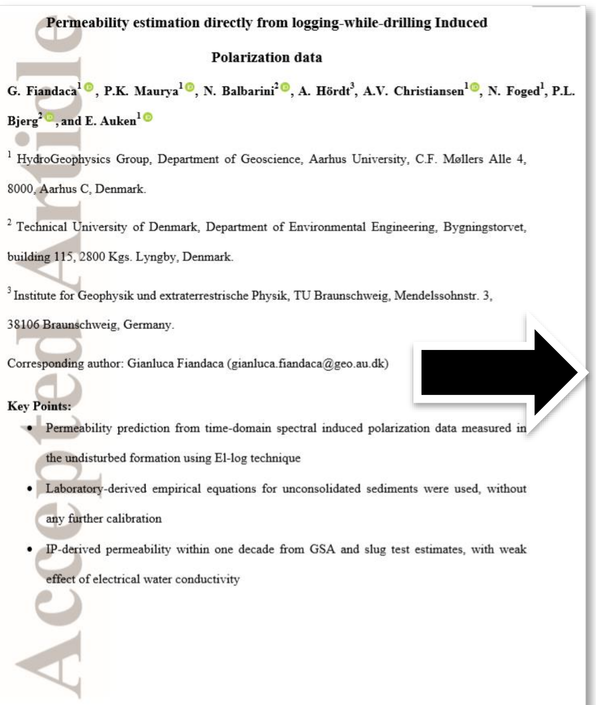
DTU Orbit





Upload

Open Access workflow


Permeability estimation directly from logging-while-drilling Induced Polarization data

G. Fiandaca[1], P.K. Maurya[1], N. Balbarini[2], A. Hördt[3], A.V. Christiansen[1], N. Foged[1], P.L. Bjerg[2], and E. Auken[1]

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[2] Technical University of Denmark, Department of Environmental Engineering, Bygningstorvet, building 115, 2800 Kgs. Lyngby, Denmark.

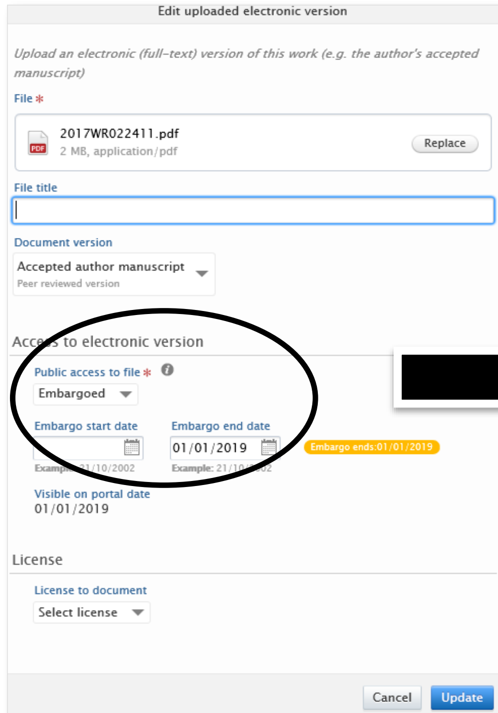
[3] Institute for Geophysik und extraterrestrische Physik, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany.

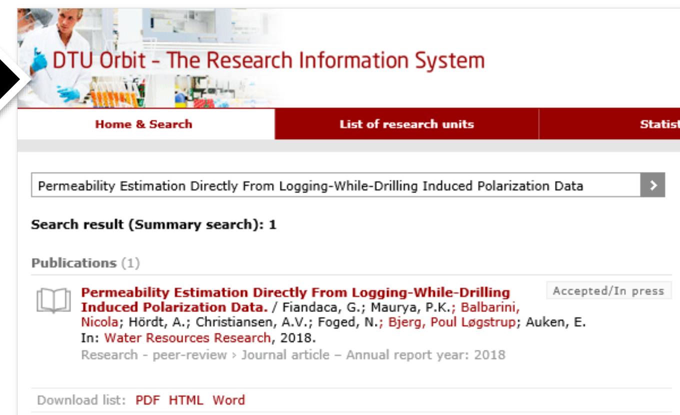
Corresponding author: Gianluca Fiandaca (gianluca.fiandaca@geo.au.dk)

Key Points:

- Permeability prediction from time-domain spectral induced polarization data measured in the undisturbed formation using El-log technique
- Laboratory-derived empirical equations for unconsolidated sediments were used, without any further calibration
- IP-derived permeability within one decade from GSA and slug test estimates, with weak effect of electrical water conductivity

Accepted Article



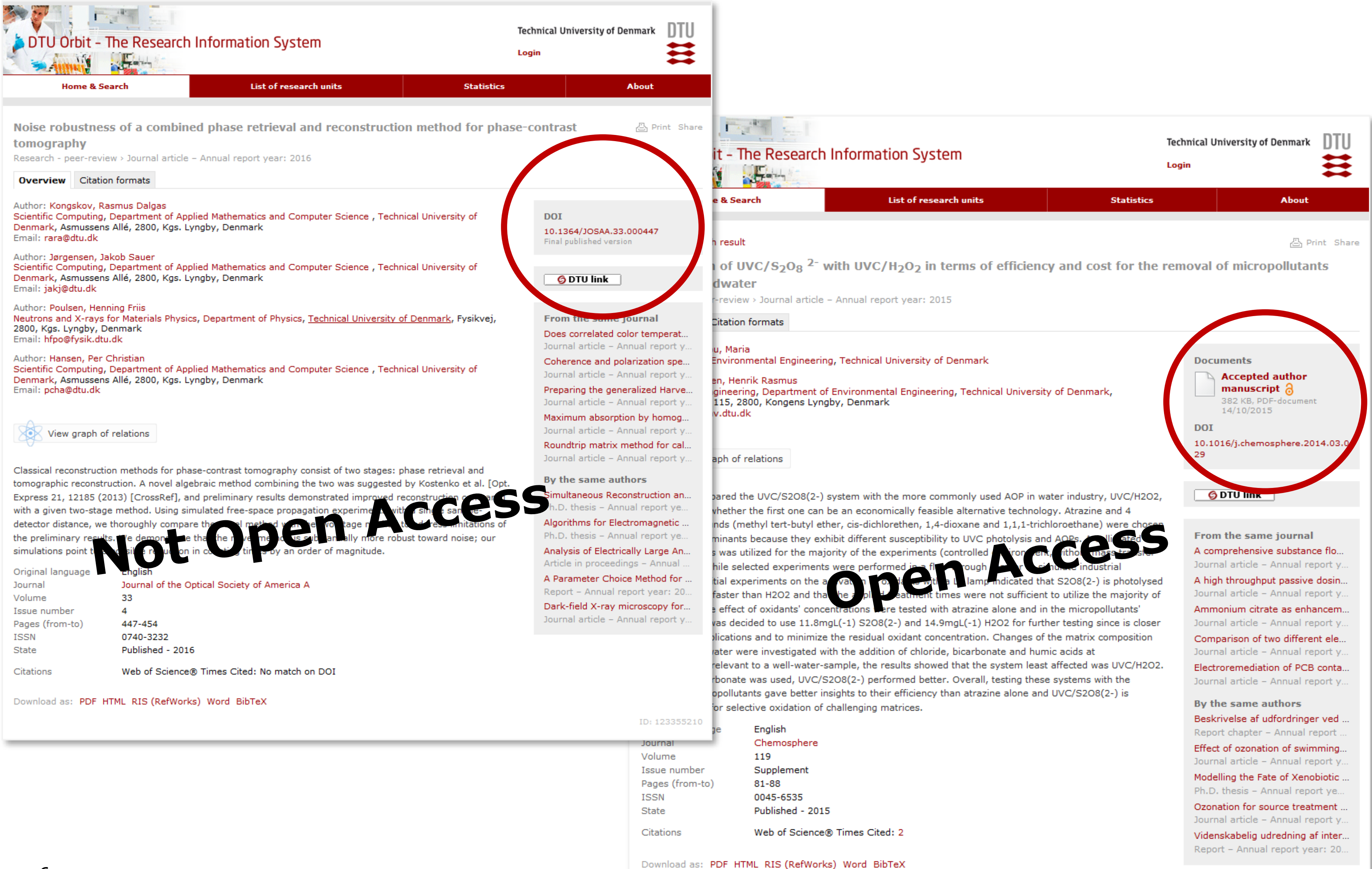


DTU researcher
Sends post-print to orbit@dtu.dk

Registration team:
Adds post-print to DTU Orbit record and checks copyright + embargo

The post-print:
Remains hidden until the embargo-period has ended. When the embargo ends, the post-print will automatically be accessible worldwide.

Green Open Access via Orbit



The post what…??

- Accepted Manuscript
- Post-print
- Accepted draft
- Accepted version
- Version 2
- Author Accepted Manuscript
- 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.

ACS Catalysis
Research Article
pubs.acs.org/acscatalysis

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,[‡,¶] Carlo Lamberti,[‡,¶] Silvia Bordiga,[*,†] Anita Godiksen,[§] Susanne Mossin,[*,§] and Pablo Beato[*,†]

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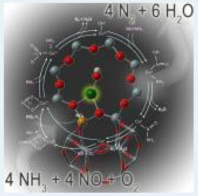
ABSTRACT: For the first time, the standard and fast selective catalytic reduction (SCR) of NO by NH_3 are described in a complete catalytic cycle that is able to produce the correct stoichiometry while allowing adsorption and desorption of stable molecules only. The standard SCR reaction is a coupling of the activation of NO by O_2 with the fast SCR reaction, enabled by the release of NO_2. According to the scheme, the SCR reaction can be divided into an oxidation of the catalyst by NO + O_2 and a reduction by NO + NH_3; these steps together constitute a complete catalytic cycle. Furthermore, both NO and NH_3 are required in the reduction, and finally, oxidation by NO + O_2 or NO_2 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 cycle. The activation energy calculated by density functional theory (DFT) indicates that the oxidation of an NO molecule by O_2 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 to NO_2.



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 N_2 by ammonia (NH_3-SCR) plays an important role in the abatement of NO_x 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 NH_3-SCR are based on vanadium oxide supported on titanium oxide, Fe-exchanged 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 NO_x, 5−10% water vapor, 5−10% O_2, hydrocarbons, CO, and CO_2. 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_x, O_2, H_2O, and NH_3 in an inert gas (N_2 and CO_2). 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 NH_3-SCR is the formation of nitrogen from NO and NH_3 according to the equation

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

Received: October 29, 2014
Revised: February 22, 2015
Published: March 19, 2015

DOI: 10.1021/cs501673g
ACS Catal. 2015, 5, 2832−2845

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,[‡,¶] Carlo Lamberti,[‡,¶] Silvia Bordiga,[*,‡] Anita Godiksen,[§] Susanne Mossin,[*,§] and Pablo Beato[*,†]

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[§]Technical University of Denmark

DTU

Interference
Ascorbic Acid De

Hongyan Bi[1] *, Ana C

[1] International Iberian Nanotechnology
[2] INESC Microsistemas e Nanotecnolo

* Correspond
Tel: + 3

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Abstract

A microfluidic sensor is devel
drug/food/beverage matrices. The surf
modified by enzyme via physisorption
microfluidic channel, enzyme-catalyze
products. The whole process is monit
oxidase and L-ascorbic acid (AA) are
feasibility of using the developed strate
matrices. A dietary supplement produ
microfluidic bio-sensor in real-sample
sensor exhibits good reproducibility,
realize, depends on low investment in
UV/vis spectrophotometer is required.
accurate, and can be potentially used f
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*

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Additional Supporting Information may be found in the online

Received May 09, 2015; Revision Received October 22, 2015;

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§]

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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.

[redacted]

A combination model with variable weight optimization for short-term electrical load forecasting [redacted]

Wei-Qin Li [a,b,*], Li Chang [c]

ARTICLE INFO

[redacted]

ABSTRACT

[redacted]

1. Introduction

[redacted]

Open Access

Open Access is a way to give free access to scientific research output, making it accessible to everybody with an Internet connection.

Digitization makes it possi...

The 3 Open Access ways:

Green:

You publish in **a traditional journal** and a prior version, the post-print version, of your article is made available free for all to use after an em-bargo period in a repository - e.g. **DTU Orbit**.

...olden:

...u publish your article in a regular **Open ...cess journal**. This involves special fees. ...metimes you can get a discount - see DTU ...ary homepage* - or you can apply for **funding** ...over your Golden Open Access expenses.

...w.bibliotek.dtu.dk/OA_Discounts

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...ublish in a traditional journal but pay a **fee** ...king your research available Open Access ...iately - bypassing the existing embargo ... Since most publishing houses allow for ...pen Access without payment, **hybrid ...ccess should be avoided.**

...een

...als support green Open Access and ...charge for you and the university ...post-print to orbit@dtu.dk

Things to consider

Quality first! Always aim to publish in the most suitable and prestigious publication chan-nels available to you. Make sure they allow for **green Open Access!**

Only choose Open Access Journals if they are considered to be on a par with traditional journals and do not involve unreasonable fees.

Danish National Strategy

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

Open Access Policies

Check the Open Access policy and embargo period of individual journals in the Sherpa-ROMEO database: www.sherpa.ac.uk/romeo. Identify Open Access journals in the Directory of Open Access Journals: www.doaj.org.

DTU Publication Policy

At DTU Open Access publishing is an important part of the publication policy. DTU publications must be easily and freely available to the widest possible audience. DTU researchers must there-fore always consider Open Access when deciding where and how to publish.

Download the policy:

www.bibliotek.dtu.dk/Publication_Policy

Green OA

When you publish in a traditional journal and the **post-print** version of your scientific article is made available online for free (after embargo period) e.g. uploaded in **DTU Orbit**

Golden OA

When you publish your article in an **Open Access journal**. This usually involves APCs (author publication charges/article processing charge)

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

pure.report

A) OPEN ACCESS: Artikler fra tidsskrifter uden postprint

A report made in Pure. Prepared by: Cæcilie Berg Heising (chei@dtu.dk), 22/08/2018 14:34

1. Publications

Analysis of Count on Publications

Type	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

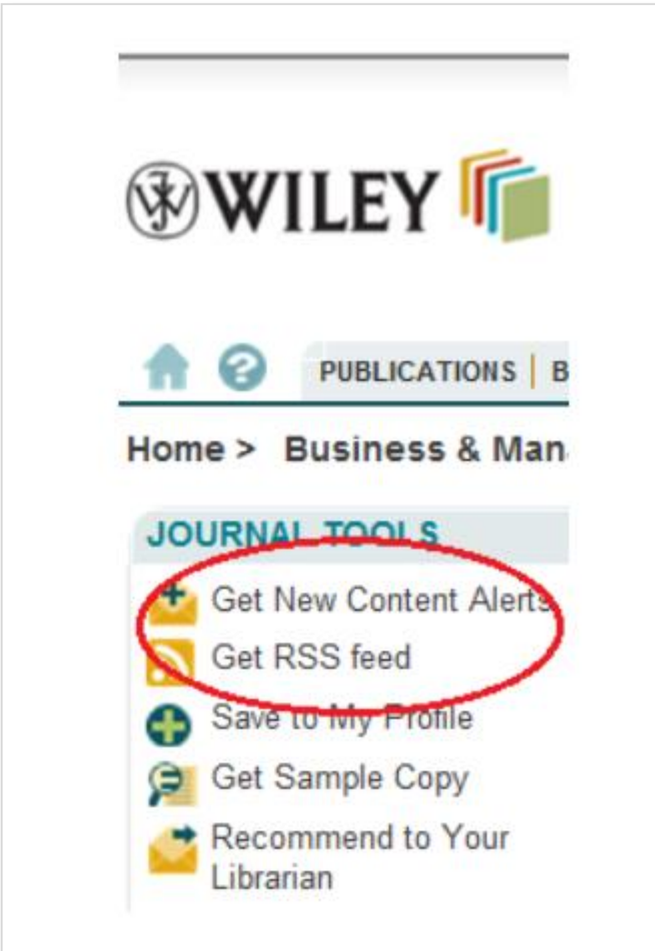
Alvarez, B., Barra, C., Nielsen, M., & Andreatta, M. (2018). Computational Tools for the Identification and Interpretation of Sequence Motifs in Immunopeptidomes. *Proteomics*, [1700252]. DOI: 10.1002/pmic.201700252

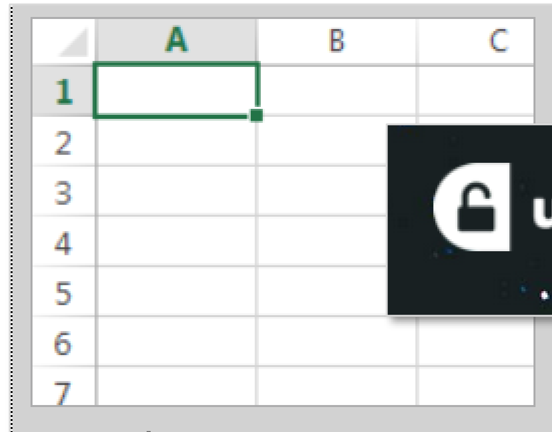
Andreatta, M., Trolle, T., Yan, Z., Greenbaum, J. A., Peters, B., & Nielsen, M. (2018). An automated benchmarking platform for MHC class II binding prediction methods. *Bioinformatics*, *34*(9), 1522-1528. DOI: 10.1093/bioinformatics/btx820

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

Forskningsresultater	
Publications	
Scientific articles with referee in ISI-indexed journals	
Scientific articles with referee	
Contributions to conferences with referee	
Books and contributions to books	
Monographs	
Contributions to books and reports	
Scientific dissertations (after 2001)	
Dr. Thesis	
Ph.d. Thesis	
Publications with no referee	
Scientific publications, articles and conference contributions with no peer-review	
Contributions indicated as popular	
Other publications	
Scientific reports	
Citations	
Citations 2010-2014 for all publications indexed in 2010-14	
Citations 2014 for all publications indexed in 2010-14	
Open Access	
Open Access to peer-reviewed journal articles and conference contributions from the previous year	

Improving workflows

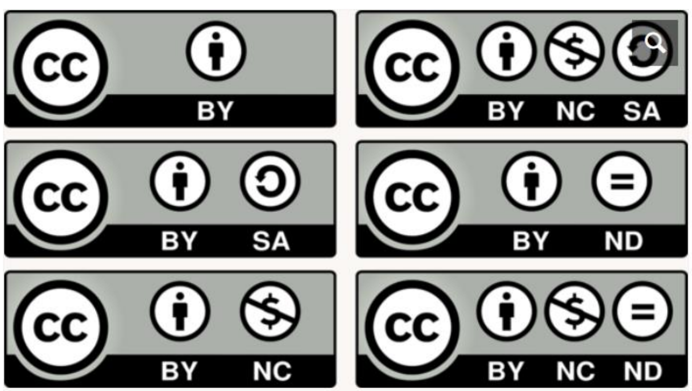




unpaywall

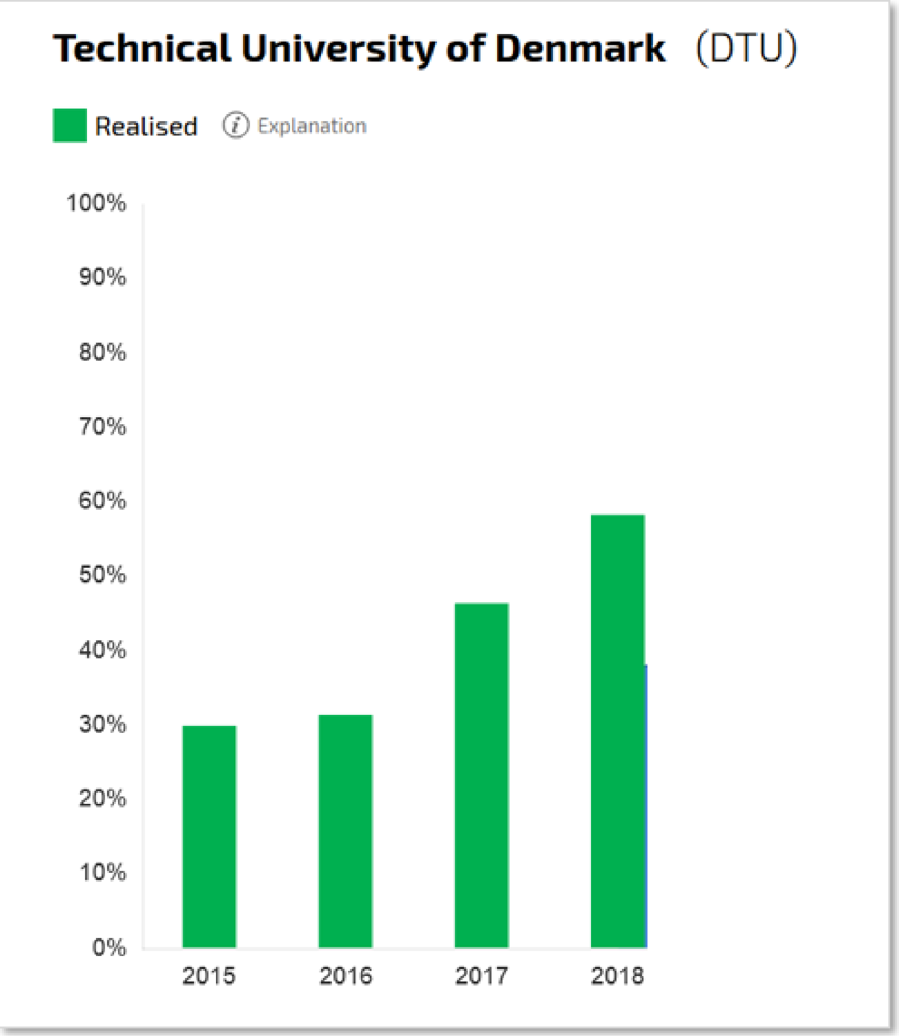
Kopernio

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?