Manuel J. Kolb
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Personal Details

Date of birth 22/6/1986 in Lauf an der Pegnitz, Germany

Research Interests

- Water adsorption structures on single-crystal surfaces
- Theoretical electrocatalysis on single-crystal transition metal surfaces
- Theoretical electrocatalysis on metal oxide surfaces

Education and Professional Experience

4/2012 – **Massachussetts Institute of Technology, Cambridge, United States**
PostDoctoral researcher in the group of Yang Shao-Horn on the topic
'Theoretical Electrochemistry on Metal Oxide Surfaces'

1/2016 – 3/2016 **Leiden Institute of Chemistry, Leiden University, The Netherlands**
Research assistant in the group of Joerg Meyer on the topic
'Interfacial Dynamics on Transition Metal Surfaces'

1/2012 – 12/2015 **Leiden Institute of Chemistry, Leiden University, The Netherlands**
PhD student in the group of Marc Koper on the topic
'Water related adsorbates on the stepped Pt(533) and Pt(553) surfaces'
Estimated completion date: March 2016

5/2014 - 7/2014 **University of Iceland, Reykjavik, Iceland**
Visiting scientist (Hydrogen adsorption structures and temperature programmed desorption simulations on stepped Pt surfaces)

10/2011 - 12/2011 **Friedrich Alexander University Erlangen-Nürnberg, Germany**
Research assistant in the DFG project 'Interaction of long living solvated electrons with adsorbates at the surface of ice'

10/2005 - 9/2011 **Friedrich Alexander University Erlangen-Nürnberg**, **Germany**
Diploma in Physics (MSc equivalent)
Diploma thesis: 'Surface vacancies and low-coordinated lattice positions on oxide surfaces'
Electives: Astronomy, Electrical Engineering, (Theoretical) Solid State Physics

Publications

Published

06/2016 Structure sensitivity of the electro-oxidation of Glycerol on Pt single crystal surfaces
Amanda Garcia, Manuel J. Kolb, Chris van Nierop-Sanchez, Jan Vos, Youngkook Kwon, Federico. Calle-Vallejo, Germano Temilioso-Filho, Marc T.M. Koper
ACS Catalysis, 2016, 6 (7), pp 4491-4500

3/2016 Double-Stranded Water on Stepped Platinum Surfaces
Manuel J. Kolb, Rachael G. Farber, Jonathan Derouin, Cansin Badan, Federico Calle-Vallejo, Ludo B.F. Juurlink, Marc T.M. Koper
Phys. Rev. Lett., Vol. 113 Issue 13, 136101

1/2016	DFT Study on the Mechanism of the Electrochemical Reduction of CO_2 Catalyzed by Cobalt Porphyrins Jing Shen, Manuel J. Kolb, Adrien J. Göttle, Marc T.M. Koper **J. Phys. Chem. C**, 2016, 120 (29), pp 15714-15721
12/2015	Incomplete Bilayer Termination of the Ice(0001) Surface Michel Bockstedte, Anja Michl, Manuel Kolb, Michael Mehlhorn, Karina Morgenstern **J. Phys. Chem. C,** 2016, 120(2), pp 1097-1109
09/2015	Initial stages of water solvation of stepped platinum surfaces Manuel J. Kolb, Jasper Wermink, Ludo B.F. Juurlink, Marc T.M. Koper, **Physical Chemistry Chemical Physics**, 2016, 18 , 3416-3422
12/2014	Why Is Bulk Thermochemistry a Good Descriptor for the Electrocatalytic Activity of Transition Metal Oxides? Federico Calle-Vallejo, Oscar A. Díaz-Morales, Manuel J. Kolb, Marc T.M. Koper **ACS Catalysis** 5(1): 869-873
4/2014	Density functional theory study of adsorption of H2O, H, O, and OH on stepped platinum surfaces. Manuel J. Kolb, Federico Calle-Vallejo, Ludo B F Juurlink, Marc T.M. Koper, **Journal of Chemical Physics** 140(13): 134708
8/2013	Why (100) Terraces Break and Make Bonds: Oxidation of Dimethyl Ether on Platinum Single-Crystal Electrodes Hongjiao Li, Federico Calle-Vallejo, Manuel J. Kolb, Youngkook Kwon, Yongdan Li, Marc T.M. Koper, **Journal of the American Chemical Society** 135(38): 14329–14338

Submitted

In preparation

Understanding the pre-OER redox processes on model RuO_2 surfaces
Reshma Rao, Manuel Kolb, Anders Pederson, Niels Bendtsen Halck, Apurva Mehta, Hoydoo Yoo, Kelsey Stoerzinger, Tejs Vegge, Ifan Stephens, Ob Chorkendorff, Yang Shao-Horn

Heterogeneous catalysis of Formaldehyde on the surface of Manganese Dioxide and the catalytic influence of water
Karthik Akkariju, Manuel Kolb, Yang Shao-Horn

Simulation of Hydrogen TPD Traces of Pt(211), Pt(221), Pt(533) and Pt(553) based on DFT calculations
Manuel J. Kolb, A. Garden, E. Skulason, L.B.F. Juurlink, H. Jonsson, M.T.M. Koper

Electronic structure of low coordinated lattice sites on MgO surfaces
Philipp Auburger, Manuel J. Kolb, Michel Bockstedte

Interaction of long living solvated electrons with adsorbates at the surface of ice
Philipp Auburger, Anja Michl, Manuel J. Kolb, Michel Bockstedte

Supervision of Students & Teaching

- Supervision and teaching of one master student and two PhD students in performing DFT calculations, resulting in three papers
- Supervision of 8 undergraduate students in multiple projects

- Teaching assistant in General and Inorganic Chemistry, Leiden University
- Teaching assistant in Theoretical Physics, Quantum Mechanics 1, University Erlangen-Nuremberg

Grants

5/2013	Computation time PRACE-2IP project (FP7 RI-283493)
Yearly, 2012-2015	Grant proposal for renewal of computation time at NWO/SurfSARA – Cartesius cluster

Cover Images

Front Cover of Physical Chemistry Chemical Physics with the Article 'Initial stages of water solvation of stepped platinum surfaces'

Front Cover of Physical Review Letters with the article „Double-Stranded Water on Stepped Platinum Surfaces“

Additional Skills

Languages	German:	Native language
	English:	Fluent in spoken and written
	French:	Basic knowledge
IT	Linux/UNIX:	User level experience, usage of HPC systems, e.g. JUROPA, Cartesius, SISU, administration of local Linux clusters and other HPC systems
	VASP 4.6-5.X:	Experience with LDA, GGA and hybrid functionals
	Quantum Espresso:	Experience with hybrid functionals (BLYP/B3LYP) in context of ice surfaces and admolecules
	ADF	Experience with ADF, ADF-BAND, REAX-FF
	CARLOS	Kinetic Monte Carlo simulations

References

Marc Koper	Leiden Institute of Chemistry, Leiden University m.koper@lic.leidenuniv.nl ; Tel : +31 (0)71 527 4250
Egill Skulason	Science Institute and Faculty of Physical Sciences, University Iceland egillsk@hi.is , Tel: +354 6948683
Joerg Meyer	Leiden Institute of Chemistry, Leiden University j.meyer@chem.leidenuniv.nl ,

Cambridge, December 8th, 2016