

## Personal Information

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 Date of birth: 11/21/1988  
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## Research Interests

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The research projects I currently work on are centered on understanding properties and reactivity of oxide-supported metal clusters and metal-supported oxide thin films. In particular, I use quantum mechanical simulations to characterize the metal/oxide interface and to investigate its catalytic properties. Recent projects include mechanistic studies of CO oxidation on Au/TiO<sub>2</sub> and CO<sub>2</sub> hydrogenation on Ru/TiO<sub>2</sub> and Cu/TiO<sub>2</sub>. I enjoy working with experimental groups, simulating spectroscopic and microscopic data.

## Work Experience

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- 10/17/13 - 03/31/14 **Post-graduate research project in the Collaborative Research Center 765 (CRC 765) of the German Research Foundation (DFG): “Multivalency as chemical organizational and operational principle”**  
 Freie Universität Berlin, Supervisor: Prof. Paulus  
 - First principle investigations of multivalent pyridine derivatives on graphene
- 06/12-08/12 **Internship**  
 Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany  
 Supervisor: Dr. Heyde  
 - Topological investigations of two-dimensional complex networks

## Education

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- 04/01/14 - present **PhD Student in Material Science and Nanotechnology**  
 Università di Milano-Bicocca, Italy, Supervisor: Prof. Pacchioni  
 - First-principle investigations of properties and reactivity of oxide-supported metal clusters and metal-supported oxide thin-films
- 10/17/13 Master thesis “Metal atom adsorption in silica bilayers” Degree: A  
 Supervisors: Prof. Paulus and Prof. Pacchioni
- 10/01/11 – **10/17/13** **Master of Science in Chemistry**, Freie-Universität Berlin, Germany Degree: A  
 Theoretical chemistry, electronic structure methods, molecular dynamics
- 10/01/08 – **08/22/11** **Bachelor of Science in Chemistry**, Ruhr-Universität Bochum, Germany  
 Physical chemistry, technical chemistry, quantum mechanics

## Scholarships

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- 04/14 - present **Early Stage Researcher Scholarship of the European FP7-ITN “CATSENSE”**  
 Università di Milano-Bicocca, Italy, Supervisor: Prof. Pacchioni
- 09/14 Trainee Grant for the COST Training School
- 10/13 - 04/14 **Doctorate Scholarship of the CRC 765, German Research Foundation (DFG)**  
 Freie Universität Berlin, Germany, Supervisor: Prof. Paulus
- 04/13 – 08/13 **ERASMUS Scholarship**  
 Università di Milano-Bicocca, Italy, Supervisor: Prof. Pacchioni

## Publications

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- 2016 (1) “Modeling of an ultra-thin silicatene/silicon-carbide hybrid film”, P. Schlexer, G. Pacchioni, *J. Phys. Condens. Matter*, 28 (2016) 364005
- (2) “Adsorption and dimerization of late transition metal atoms on the regular and defective quartz (001) surface”, P. Schlexer, G. Pacchioni, *Top. Catal.*, (2016) *in press*.
- (3) “CO adsorption on a silica bilayer supported on Ru(0001)”, P. Schlexer, G. Pacchioni, R. Włodarczyk, J. Sauer, *Surf. Sci.*, 648 (2016), 2-9
- 2015 (4) “Tuning the charge state of Ag and Au atoms and clusters deposited on oxide surfaces by doping: A DFT study of the adsorption properties of nitrogen- and niobium-doped TiO<sub>2</sub> and ZrO<sub>2</sub>”, P. Schlexer, A. Ruiz Puigdollers, G. Pacchioni, *Phys. Chem. Chem. Phys.*, 17 (2015) 22342-22360
- (5) “Gold and silver clusters on TiO<sub>2</sub> and ZrO<sub>2</sub> (101) surfaces: Role of dispersion forces”, A. Ruiz Puigdollers, P. Schlexer, G. Pacchioni, *J. Phys. Chem. C*, 119 (2015) 15381-15389
- (6) “Dense or porous packing? Two-dimensional self-assembly of star-shaped mono-, bi-, and terpyridine derivatives”, D. Trawny, P. Schlexer, K. Steenbergen, J. P. Rabe, B. Paulus, H.-U. Reissig, *ChemPhysChem*, 16 (2015) 949-953
- (7) “Characterizing crystalline-vitreous structures: from atomically resolved silica to macroscopic bubble rafts”, K. M. Burson, P. Schlexer, C. Büchner, L. Lichtenstein, M. Heyde, and H.-J. Freund, *J. Chem. Educ.*, 92 (2015) 1896-1902
- 2014 (8) “Adsorption of Li, Na, K, and Mg atoms on amorphous and crystalline silica bilayers on Ru(0001): A DFT study”, P. Schlexer, L. Giordano, G. Pacchioni, *J. Phys. Chem. C*, 118 (2014) 15884-15891
- (9) “Topological investigation of two-dimensional amorphous materials”, C. Büchner, P. Schlexer, L. Lichtenstein, S. Stuckenholtz, M. Heyde, H.-J. Freund, *Z. Phys. Chem.*, 228 (2014) 587-607

## Conferences and Presentations

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- 02/16 “Atomic structure of GeO<sub>2</sub> ultrathin films”, *Poster presentation (Abstract accepted)*, P. Schlexer, A. Lewandowski, K. Burson, C. Büchner, W.-D. Schneider, M. Heyde, G. Pacchioni, H.-J. Freund, Gordon Research Conference, Pisa, Italy
- 10/16 “CO oxidation on Au nanoparticles supported on TiO<sub>2</sub> anatase (101). A Mars-van Krevelen mechanism?”, *Poster presentation*, P. Schlexer, G. Pacchioni, IV Congresso Nazionale della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana, Pisa, Italy - **Best poster award** -
- 09/16 “Reactivity and anchoring of supported Au clusters”, *Oral presentation*, P. Schlexer, G. Pacchioni, FP7-ITN “CATSENSE” meeting, Varese, Italy
- 03/16 “Adsorption and dimerization of late transition metal atoms on the quartz (001) surface”, *Oral presentation*, P. Schlexer, G. Pacchioni, FP7-ITN “CATSENSE” meeting, Bruges, Belgium
- 02/16 “CO adsorption at interfaces between metals and metal-oxides”, *Oral presentation*, P. Schlexer, G. Pacchioni, CAMD/CINF Group Meeting, Lyngby, Denmark
- 12/15 “Effect of vdW-forces and doping on the cluster-support interaction: the case of Ag and Au clusters on titania”, *Poster presentation*, P. Schlexer, A. Ruiz Puigdollers, G. Pacchioni, III Congresso Nazionale della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana, Rome, Italy
- 11/15 “Tuning the charge state and structure of small Au clusters on titania anatase and rutile: The effect of defects”, *Oral presentation*, P. Schlexer, G. Pacchioni, FP7-ITN “CATSENSE” meeting, Birmingham, UK
- 09/15 “Charging of small metal clusters on titania - The effect of doping”, *Oral presentation*, P. Schlexer, G. Pacchioni, European Conference of Surface Science (ECOSS) 31, Barcelona, Spain
- 05/15 “Adsorption of sub-nanometer Ag and Au clusters on the defective titania anatase (101) surface”, *Oral presentation*, P. Schlexer, G. Pacchioni, FP7-ITN “CATSENSE” meeting, Tel Aviv, Israel
- 11/14 “Interaction of metal atoms with SiO<sub>2</sub> bilayers and the TiO<sub>2</sub> anatase (101) surface”, *Oral presentation*, P.

- Schlexer, G. Pacchioni, FP7-ITN “CATSENSE” meeting, Birmingham, UK
- 06/14 “Adsorption of Li, Na and K atoms on silica-bilayers supported on Ru(0001)”, *Poster presentation*, P. Schlexer, G. Pacchioni, Cluster Surface Interaction Workshop, Varese, Italy
- 09/12 “Topological investigations of two-dimensional complex networks”, *Oral presentation*, P. Schlexer, C. Büchner, L. Lichtenstein, S. Stuckenholtz, M. Heyde, H.-J. Freund, Chemical Physics Workshop of the Fritz-Haber-Institute, Döllnsee, Germany
- 03/12 Frühjahrssymposium of the JungChemikerForum (JCF) of the Gesellschaft Deutscher Chemiker (GDCh), Rostock, Germany

## References

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Prof. Gianfranco Pacchioni, Email: [gianfranco.pacchioni@mater.unimib.it](mailto:gianfranco.pacchioni@mater.unimib.it)  
Department of Material Science, Università di Milano-Bicocca, Italy

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Department of Physics, Katholieke Universiteit Leuven, Belgium

Dr. Markus Heyde, Email: [heyde@fhi-berlin.mpg.de](mailto:heyde@fhi-berlin.mpg.de)  
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

## Technical and Complementary Skills

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Computer skills	Proficient with VASP, experience with Crystal, ASE, ASAP, GPAW, Gaussian Proficient with Linux, Mac OS, Windows Competent with Bash scripting, Python, Gnuplot, Latex, Office Competent with HTML/CSS ( <a href="http://lowspin.de">lowspin.de</a> )
Training schools	14-19/08/16: “Electronic Structure Theory and Materials Design”, Lyngby, Denmark 07-11/09/15: “Physics and Chemistry of Nano-clusters”, Bruges, Belgium 08-11/09/14: “Advanced Experimental Methods for Energy Materials Characterization”, Delmenhorst, Germany
Complementary courses	10/06/16: “Grant writing”, Università di Milano-Bicocca 26-27/11/13: “Team leader: Starting with success!”, Freie Universität Berlin
Teaching	11/16-present: Supervision of a visiting PhD student, Università di Milano-Bicocca
Languages	English (fluent), German (fluent), Italian (fluent), Spanish (basics), French (basics)

## Visiting PhD

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15/01/16-15/04/16	Supervisors: Prof. Schiøtz and Prof. Chorkendorff, Danmarks Tekniske Universitet - Size dependence of the melting temperature of Pt and Au nanoparticles: A combined molecular dynamics and transmission electron microscopy study
06/01/15-06/04/15	Supervisor: Prof. Lievens, Katholieke Universiteit Leuven - Deposition of sub-nanometer Ag clusters on quartz and characterization via photo-luminescence measurements
15-23/12/14	Supervisor: Prof. Sauer, Humboldt University Berlin - First principle investigations of CO adsorption on Ru-supported silica bilayers

## Miscellaneous

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Voluntary activities	06/15 - present: PhD student representative in the FP7-ITN “CATSENSE” 07/14 - present: PhD student representative, Università di Milano-Bicocca 2012: Student representative in the commission for elaboration and adaptation of framework examination regulations for the Bachelor/Master chemistry study path, Freie Universität Berlin 2011 - 2013: Member of the student association initiative in chemistry, Freie Universität Berlin
Outreach activities	Science blog: <a href="http://lowspin.de">lowspin.de</a>
Memberships	Gesellschaft Deutscher Chemiker (GDCh), American Chemical Society (ACS)