

# Welcome to Bernd Meyer's Group

**Note that the Meyer Group has moved to Universität Erlangen-Nürnberg**

## Scientific Interests:

Our main research interest is the investigation of various physical and chemical problems in surface and materials science using density-functional based ab-initio methods. For the study of structural and dynamic properties surfaces, adsorbates and interfaces we use the MBPP Mixed-Basis Pseudopotential code (which has been and is still developed in our group in close collaboration with other scientific partners) and the CPMD Car-Parrinello Molecular Dynamics program package.

## Surface Science / Heterogeneous Catalysis

Our group takes part in two projects (C6 and C11) in the Bochum collaborative research center (Sonderforschungsbereich) SFB 558 "Metal-Substrate Interactions in Heterogeneous Catalysis". The SFB 558 is focused on the study of the methanol synthesis reaction from synthesis gas ( $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{H}_2$ ) over ZnO- and Cu/ZnO-based catalysts. Specific investigations are being performed in the following fields:

- structure and composition of the catalyst surfaces at reaction conditions
- atomistic origin of morphological changes of oxide supported metal clusters ("strong metal-support interaction")
- structure and properties of adsorbates (in particular water) on oxide surfaces
- calculation of STM images

## Materials Science

- intermetallic compounds: properties of atomic defects, mechanisms of self-diffusion
- ferroelectric materials: modification of ferroelectricity at surfaces and interfaces (domain walls), critical thickness of ferroelectric thin films, ferroelectric properties of artificially layers perovskite oxides
- atomic and electronic structure of metal/oxide interfaces

## Method Development

- mixed-basis pseudopotential code (MBPP) for periodic systems
  - parametrization of tight-binding models and bond-order potentials from full DFT calculations
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## Curriculum Vitae:

- 1987-1994:  
Student of Physics and Mathematics at the University of Stuttgart
- 1993-1994:  
Diploma thesis at the Max-Planck-Institut für Metallforschung in Stuttgart under the supervision of Prof. Manfred Fähnle. Research project: "A mathematical scheme for the calculation of valence wave functions in the ionic core region in pseudopotential methods"
- 1995-1998:  
PhD in Physics at the Max-Planck-Institut für Metallforschung in Stuttgart under the supervision of Prof. Manfred Fähnle. Research project: "Development of a new ab-initio mixed-basis pseudopotential code and investigation of atomic defects in molybdenum and intermetallic compounds"
- 1995-1996:  
DAAD scholarship for a one year stay at the Ames Laboratory (USDOE) and the Department of Physics, Iowa State University, Ames, IA, USA, in the group of Prof. Kai-Ming Ho

- 1999-2000:  
Postdoc in the group of Prof. David Vanderbilt at the Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, USA
  - 2000-today:  
Research Assistant (Habilitation) at the Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum in the group of Prof. Dominik Marx
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## Publications list

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## Group members

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### Collaborations:

Within the collaborative research center SFB 558:

- Theoretical Chemistry:  
Prof. Dr. Volker Staemmler,  
Dr. Karin Fink,  
Prof. Dr. Christof Hättig (Teilprojekte C1, C2, C11)
- Physical Chemistry:  
Prof. Dr. Christof Wöll,  
Dr. Franziska Traeger,  
Dr. Yuemin Wang,  
Dr. Alexander Birkner (Teilprojekte A4, C7, C8)
- Technical Chemistry:  
Prof. Dr. Martin Muhler,  
Prof. Dr. Olaf Hinrichsen (Teilprojekt A1)

Outside the collaborative research center SFB 558:

- Prof. Dr. Christian Elsässer, Fraunhofer-Institut für Werkstoffmechanik, Freiburg, Germany  
Method development: mixed-basis pseudopotential code, parametrization of tight-binding models and bond-order potentials from full DFT calculations Applications: Ferroelectric materials, atomic and electronic structure of metal/oxide interfaces (Schottky barriers)
- Dr. Ralf Drautz, Materials Modelling Laboratory, University of Oxford, UK  
Method development: parametrization of tight-binding-models and bond-order potentials from full DFT calculations
- Dr. Frank Lechermann, Centre de Physique Theorique (CPHT), Ecole Polytechnique, Paris, France  
Method development and implementation of new features into the mixed-basis pseudopotential code
- Prof. Dr. Ulrike Diebold, Physics Department, Tulane University, New Orleans, LA, USA  
Structure and dynamics of water layers on metal oxide surfaces (Car-Parrinello molecular dynamics simulations, calculation of STM images), kinetics of metal deposition on oxide surfaces