

# List of Publications

## Papers

- [1] S. Joshi, F. Bischoff, R. Koitz, D. Ecija, K. Seufert, A. P. Seitsonen, J. Hutter, K. Diller, J. I. Urgel, H. Sachdev, J. V. Barth, and W. Auwärter. Control of Molecular Organization and Energy Level Alignment by an Electronically Nanopatterned Boron Nitride Template. *ACS Nano*, 2013, doi:10.1021/nn406024m.
- [2] R. Koitz, A. P. Seitsonen, M. Iannuzzi, and J. Hutter. Structural and Electronic Properties of a Large-Scale Moire Pattern of hexagonal Boron Nitride on Cu(111) studied with Density Functional Theory. *Nanoscale*, 5:5589, 2013.
- [3] J. Gomez Diaz, Y. Ding, R. Koitz, A. P. Seitsonen, M. Iannuzzi, and J. Hutter. Hexagonal Boron Nitride on Transition Metal Surfaces. *Theoretical Chemistry Accounts*, 132:1350, 2012.
- [4] S. Joshi, D. Ecija, R. Koitz, M. Iannuzzi, A. P. Seitsonen, J. Hutter, H. Sachdev, S. Vijayaraghavan, F. Bischoff, K. Seufert, J. V. Barth, and W. Auwärter. Hexagonal Boron Nitride on Cu(111): An electronically corrugated monolayer. *Nano Lett*, 12:5821, 2012.
- [5] R. Koitz, T. M. Soini, A. Genest, S. B. Trickey, and N. Rösch. Scalable properties of metal clusters: A comparative study of modern exchange-correlation functionals. *J Chem Phys*, 137:034102, 2012.
- [6] R. Koitz, T. M. Soini, A. Genest, S. B. Trickey, and N. Rösch. Structure-Dependence of the Magnetic Moment in Small Palladium Clusters: Surprising Results from the M06-L Meta-GGA Functional. *Int J Quantum Chem*, 112:113–120, 2011.

## Current/Submitted Manuscripts

- [1] S. Barman, A. Khutia, R. Koitz, O. Blacque, H. Furukawa, M. Iannuzzi, O. M. Yaghi, C. Jainak, J. Hutter, and H. Berke. Synthesis and hydrogen adsorption properties of internally polarized 2,6-azulenedicarboxylic acid based MOFs. *in preparation*, 2013.

## Posters and Presentations

- [1] R. Koitz. TTPB on Metallic and Liquid Surfaces: Towards Network Formation, 2013. Seminar Presentation.
- [2] R. Koitz, A. P. Seitsonen, M. Iannuzzi, and J. Hutter. Large-Scale Moiré Patterns of hexagonal Boron Nitride on Cu(111): DFT Studies of Structural and Electronic Properties. Talk at DPG Spring Meeting, Regensburg, March 2013.
- [3] R. Koitz, M. Iannuzzi, A. Seitsonen, and J. Hutter. Hexagonal Boron Nitride on Nickel and Copper Surfaces. Poster at Swiss Chemical Society Fall Meeting, 2012.
- [4] R. Koitz. Semiempirical Methods: Tight-binding and beyond, 2011. Seminar Presentation.