



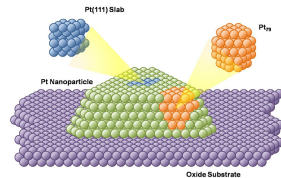
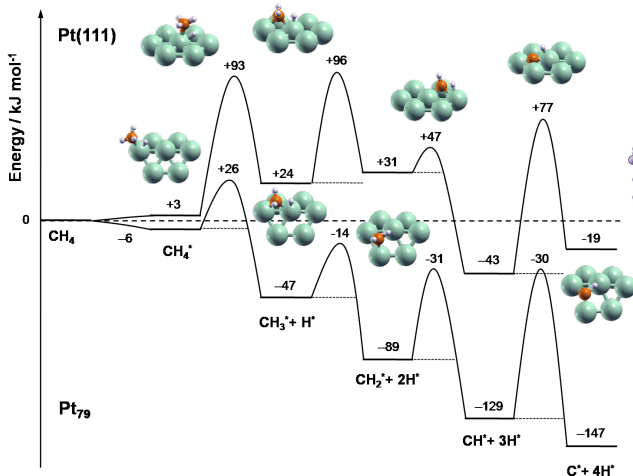
# Chemistry and Material Science on the Computer: Wavefunctions, Orbitals, and Electron Densities in Spectroscopy, Catalysis and Synthesis

Görling Group

Chair of Theoretical Chemistry

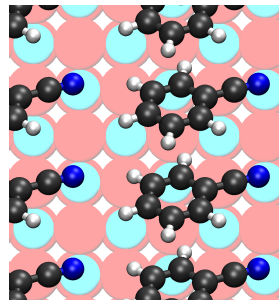
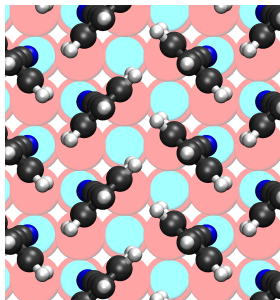
Development and application of quantum chemical methods  
for investigation of  
molecules, clusters, surfaces, and solids  
with respect to

- energetics and structure
- reactivity (catalysis)
- electronic structure (orbitals, band structures, STM)
- spectroscopy (UV/Vis, IR, NMR, non-linear optical properties)

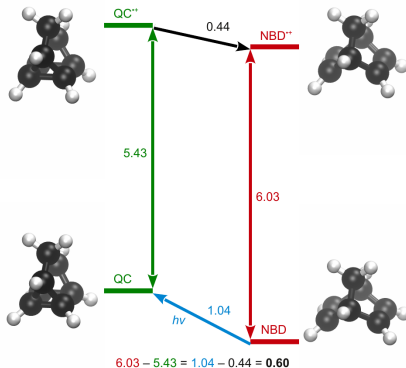


Collaboration with groups of J. Libuda and H.-P. Steinrück

## Self-organized layers of benzonitrile on MgO(100) depending on coverage

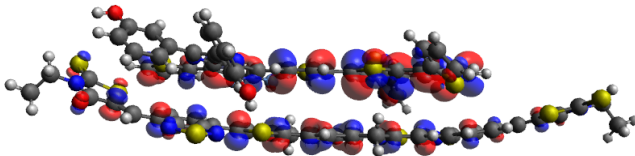


Collaboration with groups of J. Libuda, A. Schneider, S. Maier  
within DFG research unit funCOS



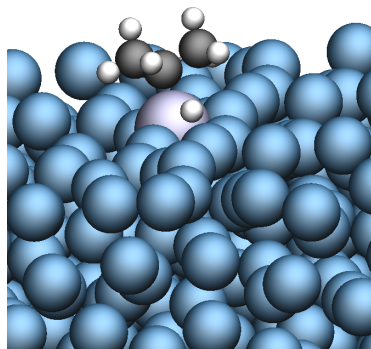
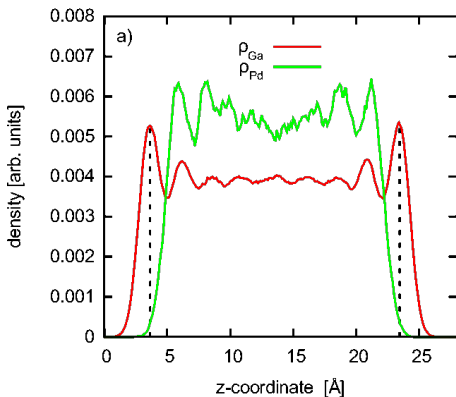
Collaboration with groups of A. Hirsch, J. Libuda,  
H.-P. Steinrück, and J. Bachmann

## Development of new donor-acceptor units



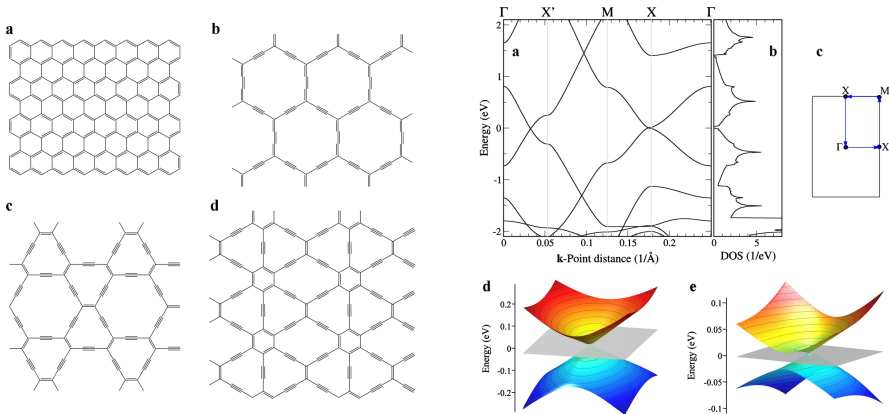
Collaboration with group of C. Brabec

## Liquid Pd/Ga or Rh/Ga mixtures as catalyst for hydrocarbon de-hydrogenation









Collaboration with groups of P. Wasserscheid and H. P. Steinrück

## Alternatives to graphene with equally amazing electronic properties



within DFG collaborative research center 953



- 1  Structure and energetics of novel carbon allotropes Christian Neiß
- 2  New 2D materials Christian Neiß
- 3  Organic molecules on metal oxide surfaces Lukas Fromm
- 4  Materials for photovoltaics and energy storage  
Stefan Frühwald / Lukas Fromm
- 5  Liquid metal catalysis (ab-initio dynamics simulations) Sven Maisel
- 6  Test of novel electronic structure methods  
Daniel Schmidtel / Jannis Erhard / Simon Kalass