Department Chemie und Pharmazie

Interdisziplinäres Zentrum für "Interface Controlled Processes"

Friedrich-Alexander-Universität Erlangen-Nürnberg

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

Görling Group

Chair of Theoretical Chemistry

Research

Development and application of quantum chemical methods

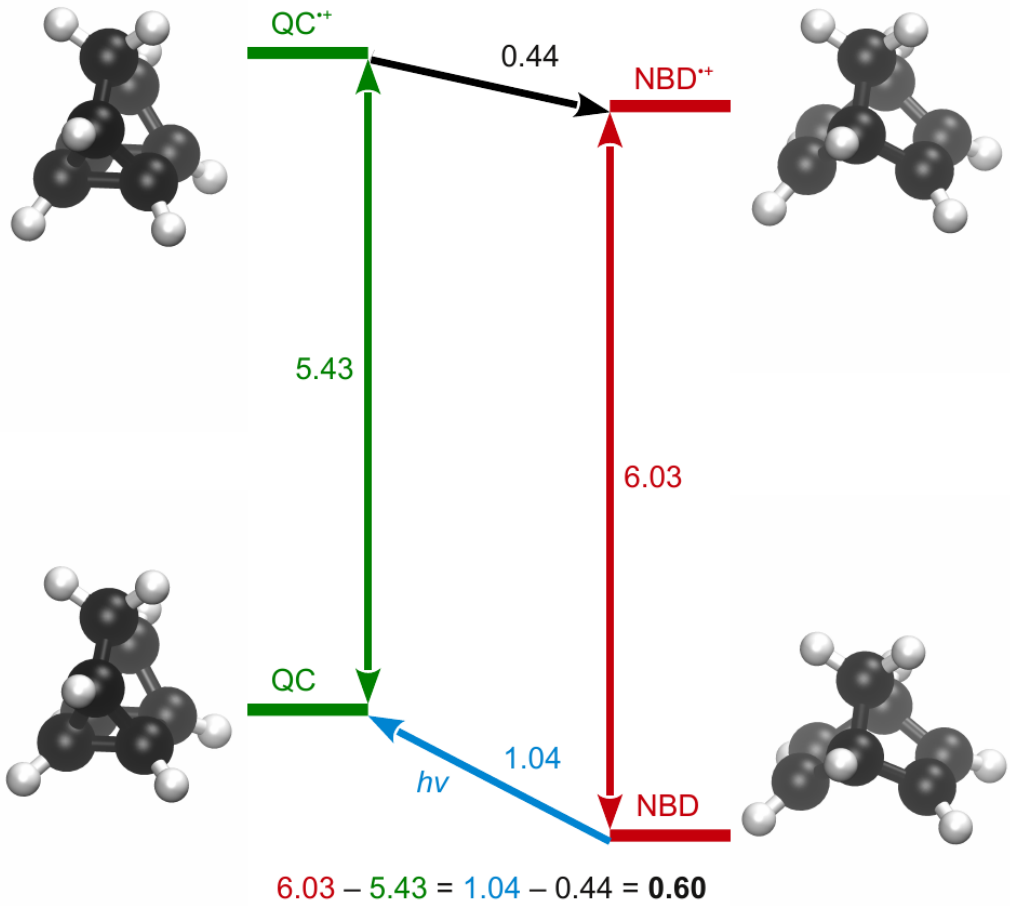
for investigation of

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)

Chemical Energy Storage

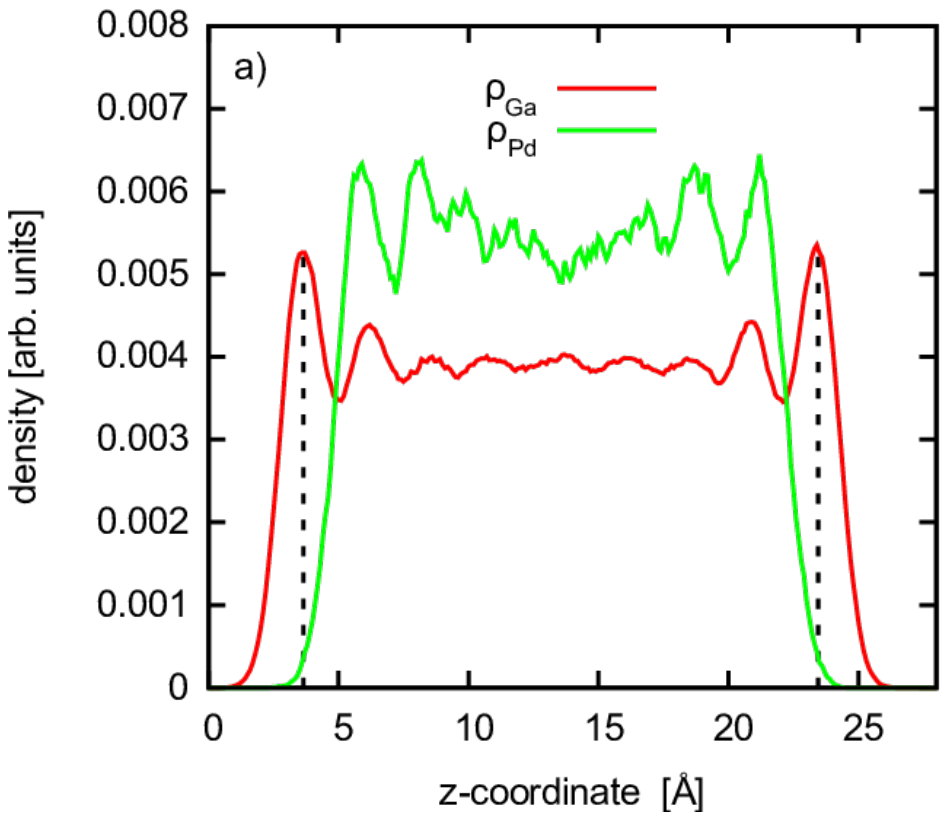


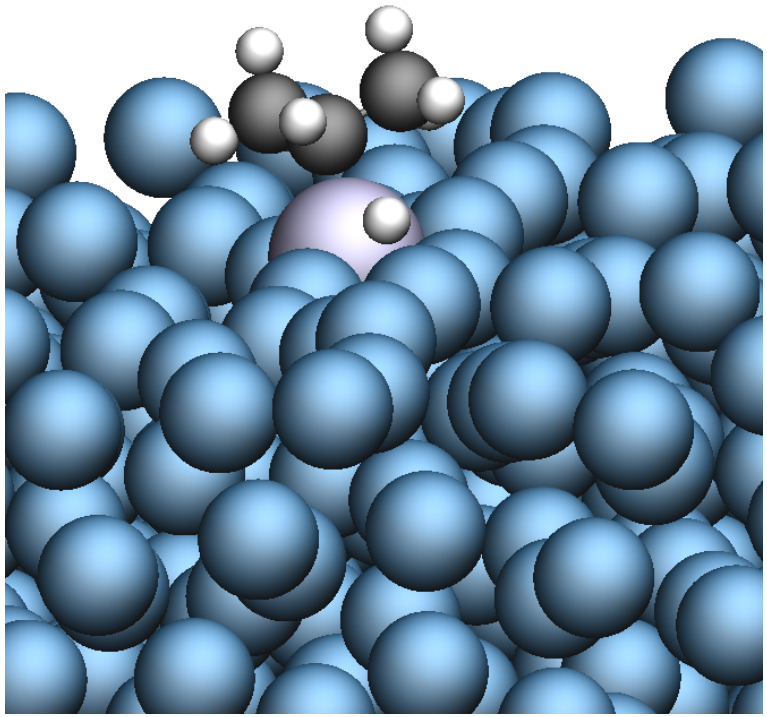
6.03 – 5.43 = 1.04 – 0.44 = **0.60**

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

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

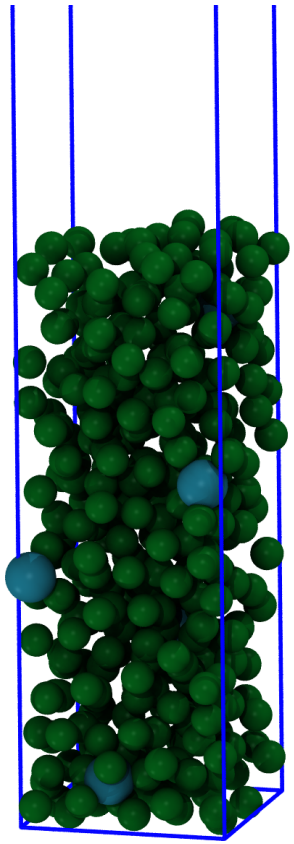
Methodology: Machine-learned force field trained on-the-fly by DFT data



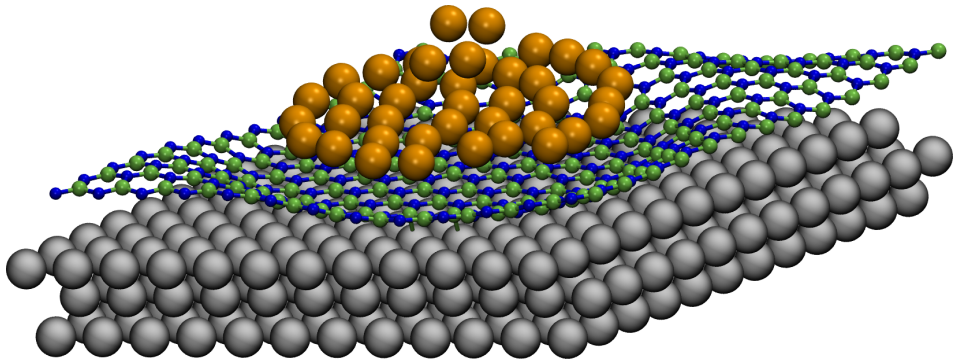


Within DFG collaborative research center 1452 "Catalysis at liquid interfaces"

Influence of dynamic processes



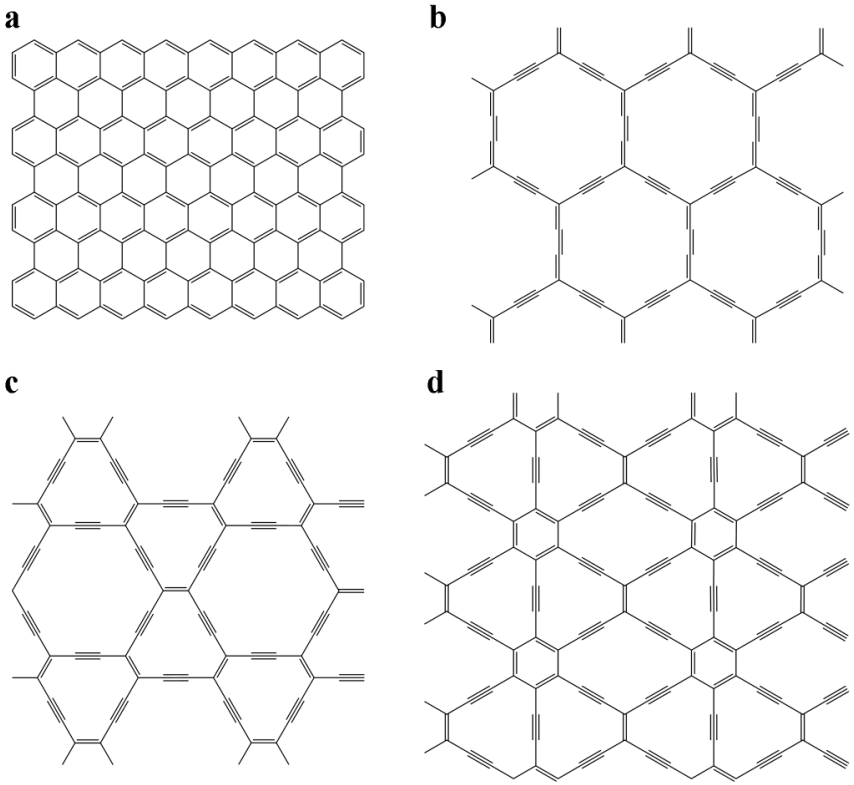
Calculation of diffusion coefficient to interpret results from neutron diffraction

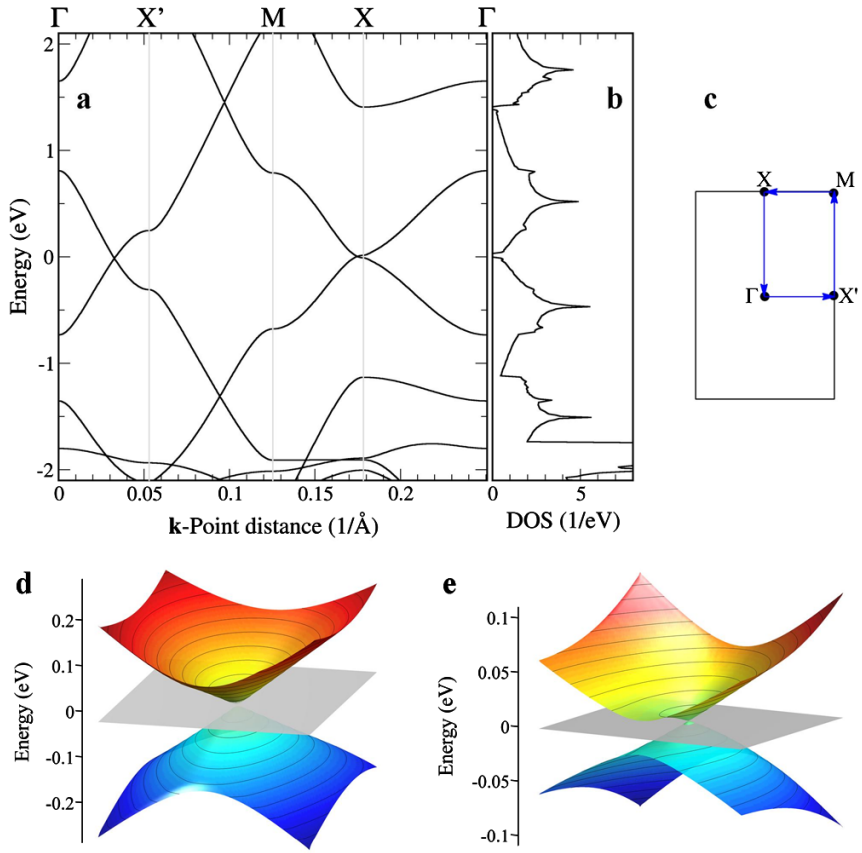


Structure formation in komplex systems

New carbon allotropes: graphynes

Alternatives to graphene with equally amazing electronic properties





Within DFG collaborative research center 953 "Synthetic carbon allotropes"

Topics Bachelor Thesis

1. New carbon-rich molecules and materials — Christian Neiß
2. New 2D materials — Joachim Paier
3. Organic molecules and ionic liquids on metal surfaces — Julien Steffen
4. Liquid metal catalysis (ab-initio dynamics simulations) — Andreas Mölkner
5. Test of novel electronic structure methods — Steffen Fauser