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

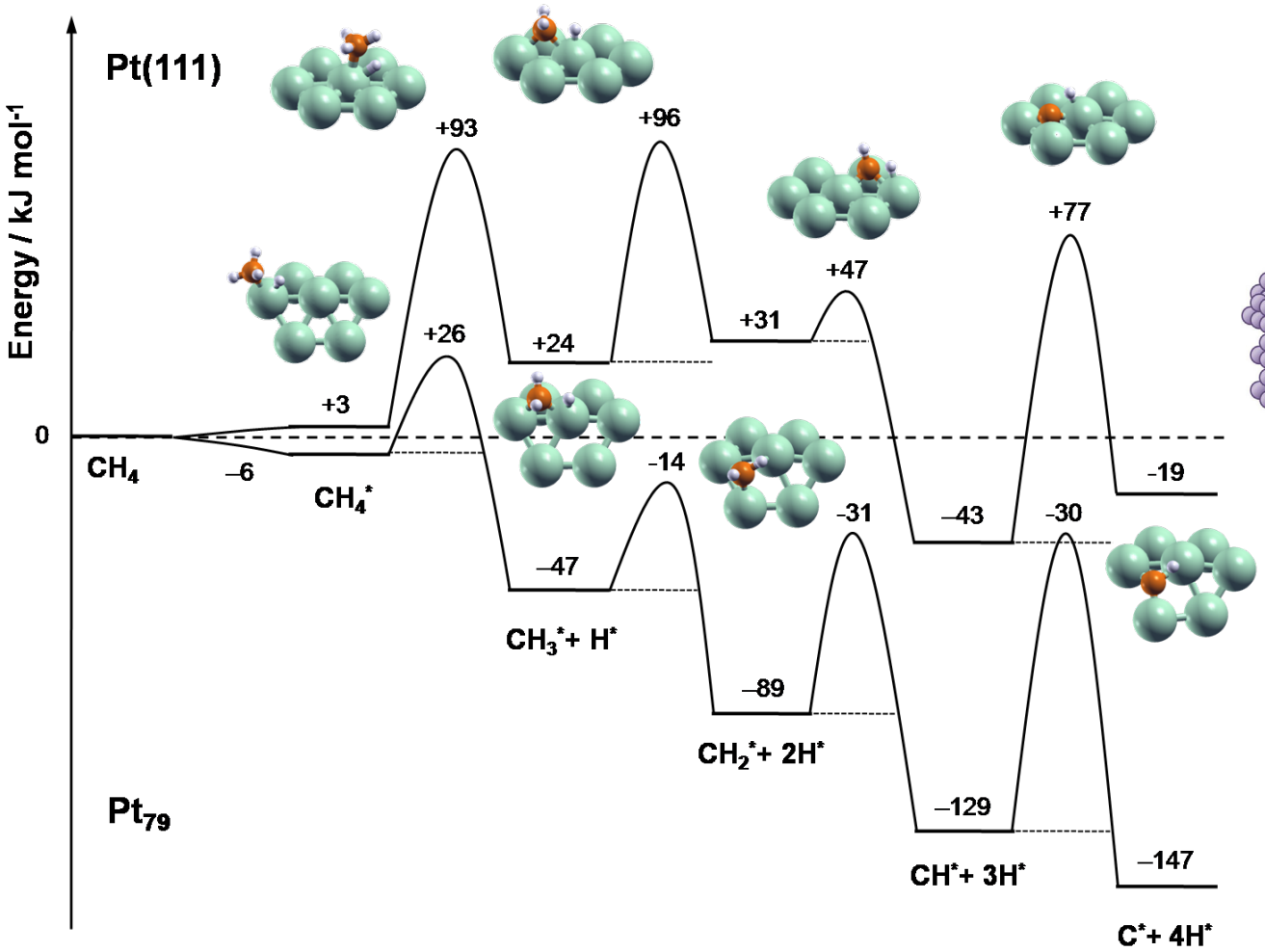
for investigation of

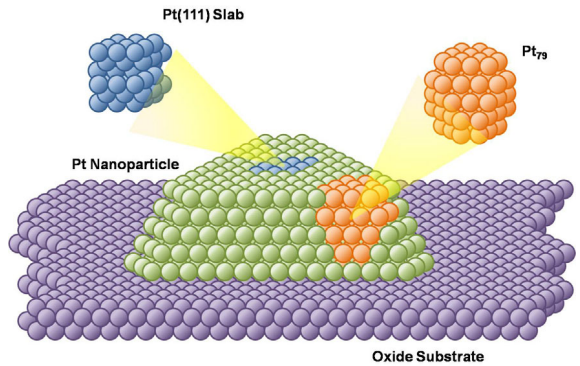
molecules, clusters, surfaces, and solids

with respect to

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

Methane decomposition on platinum surfaces and nanocrystallites

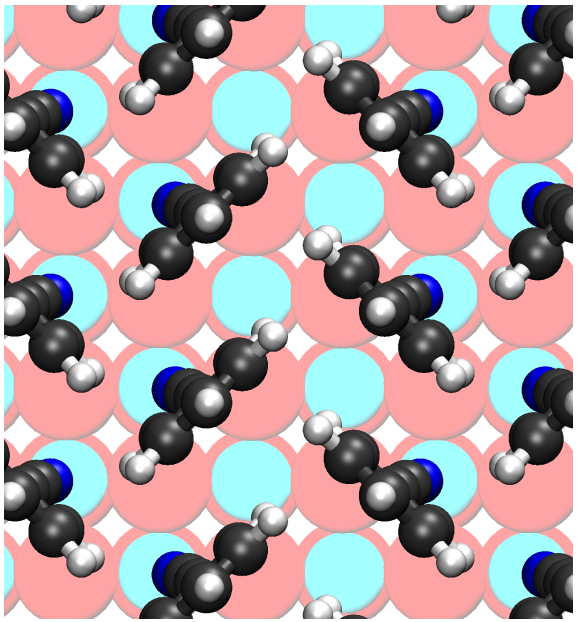


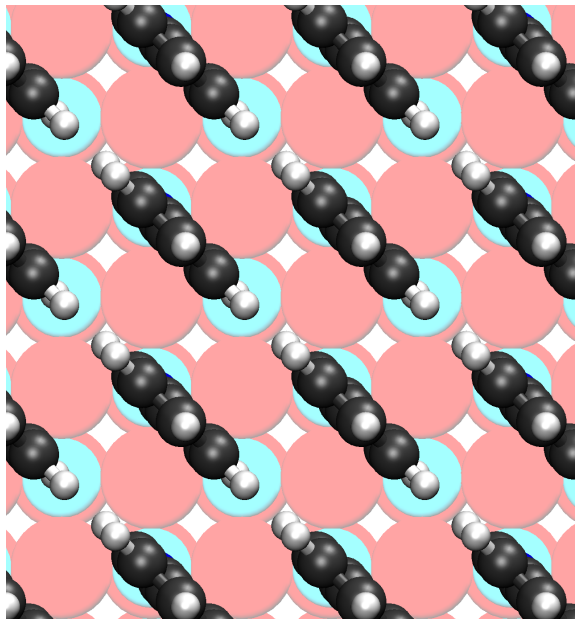


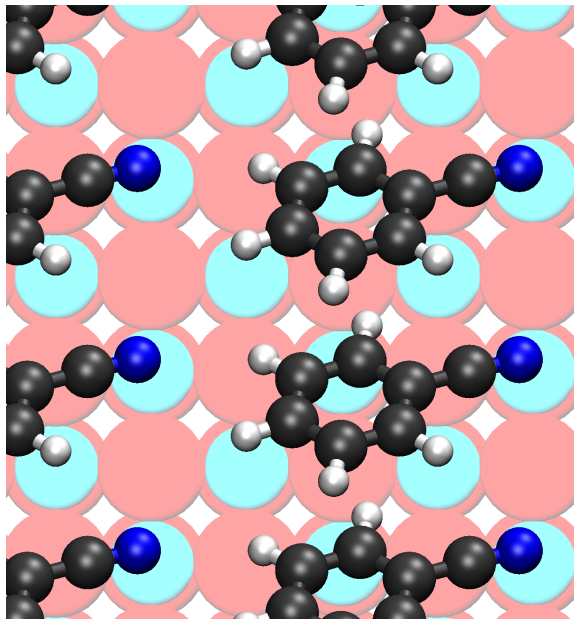
Collaboration with groups of J. Libuda and H.-P. Steinrück

Adsorption of benzonitrile on MgO

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

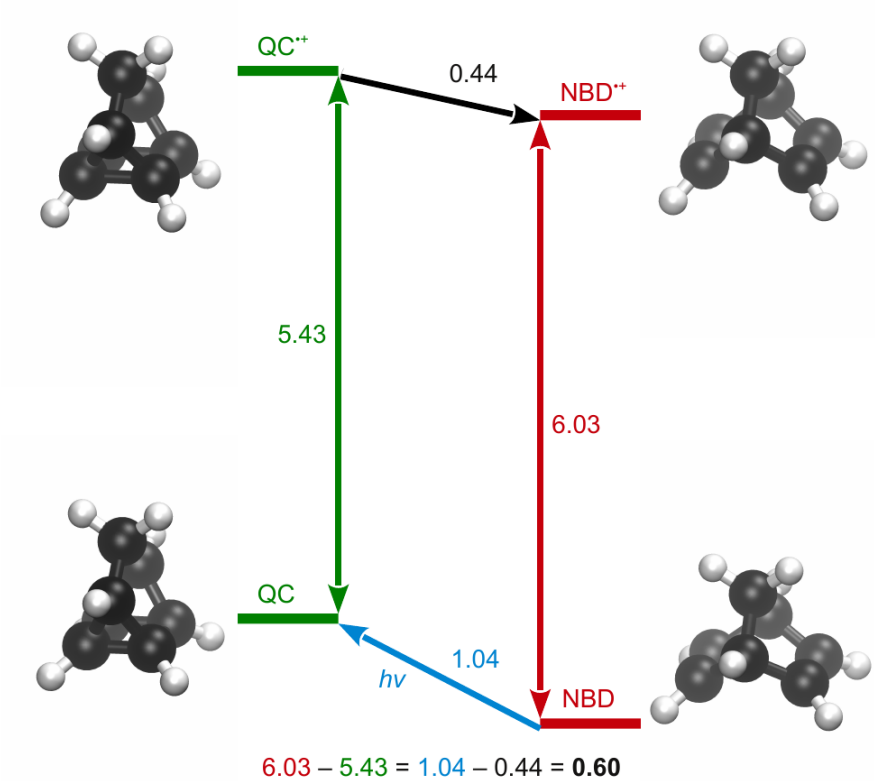






Collaboration with groups of J. Libuda, A. Schneider, S. Maier within DFG research unit funCOS

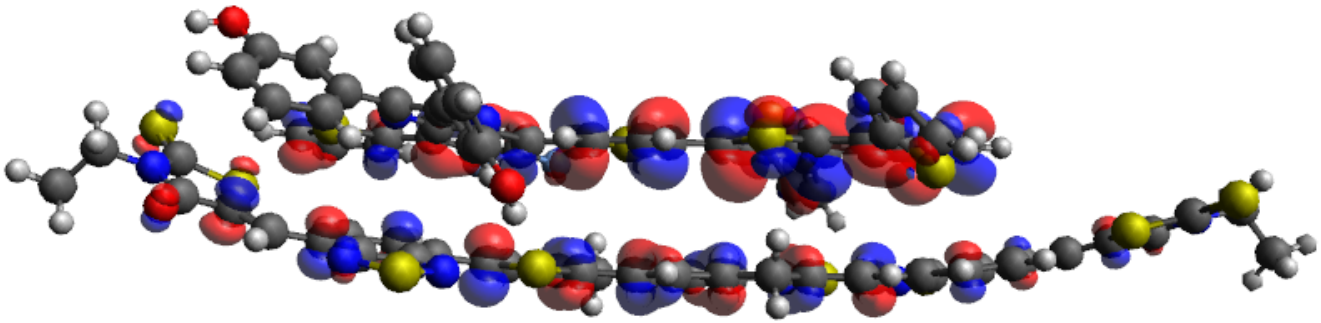
Chemical Energy Storage



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

New materials for photovoltaics

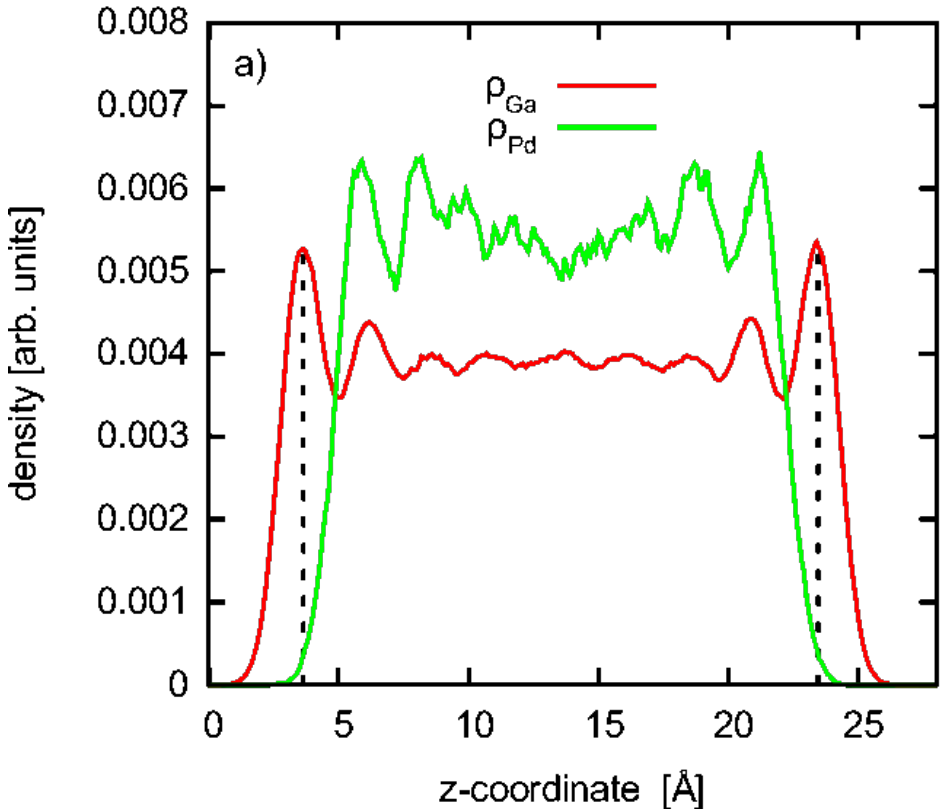
Development of new donor-acceptor units

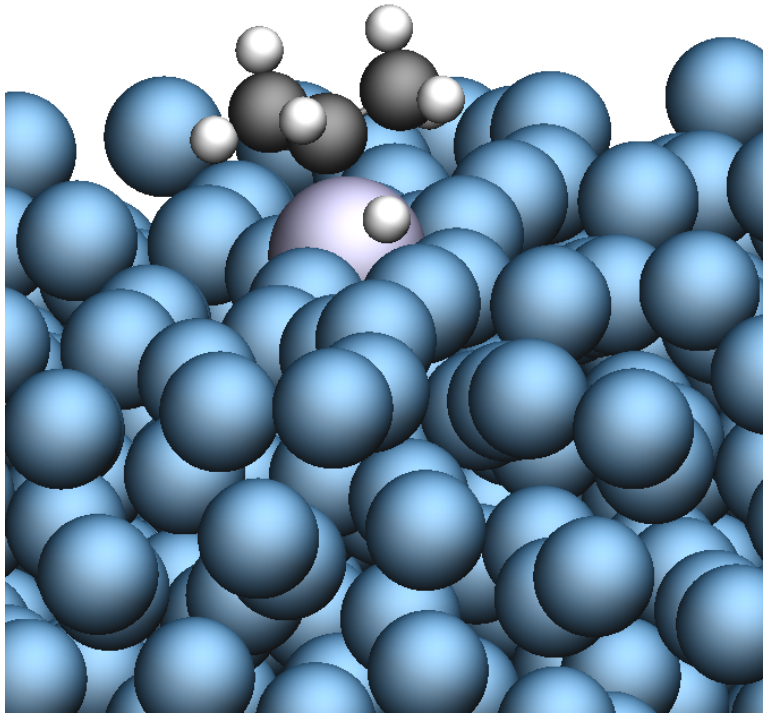


Collaboration with group of C. Brabec

Catalysis with liquid metals

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

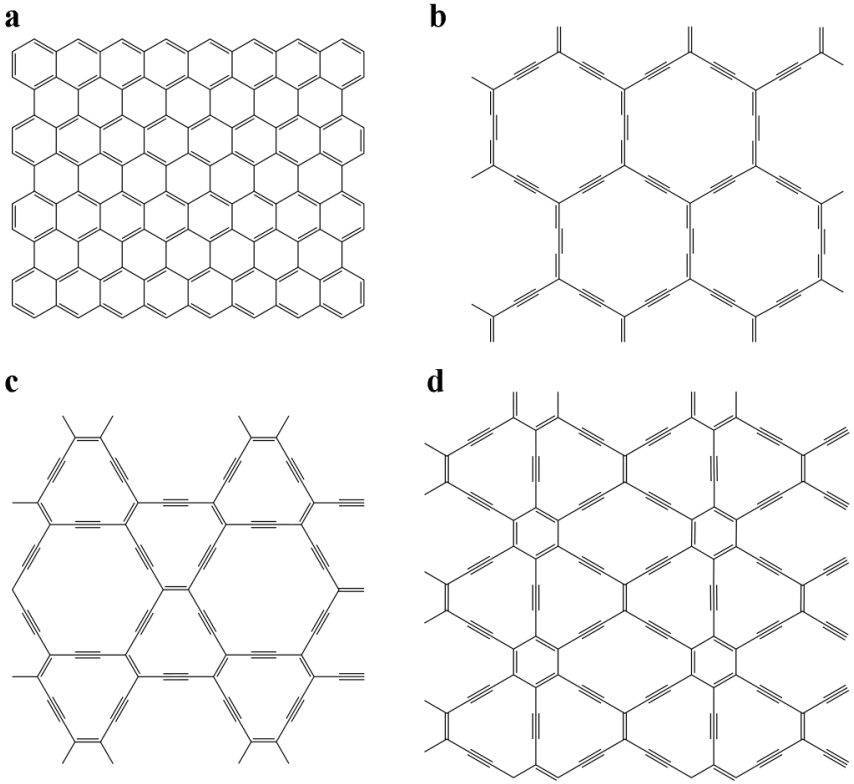


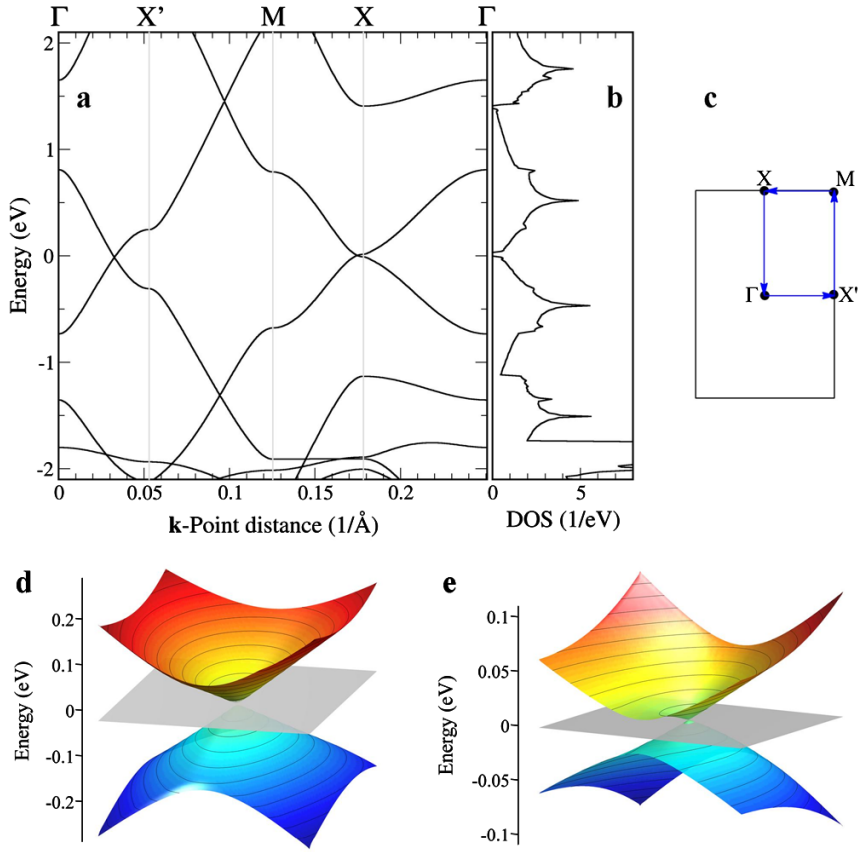


Collaboration with groups of P. Wasserscheid and H. P. Steinrück

New carbon allotropes: graphynes

Alternatives to graphene with equally amazing electronic properties





within DFG collaborative research center 953

Topics Bachelor Thesis

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
Adrian Thierbach / Jannis Erhard / Simon Kalass / Steffen Fauser