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

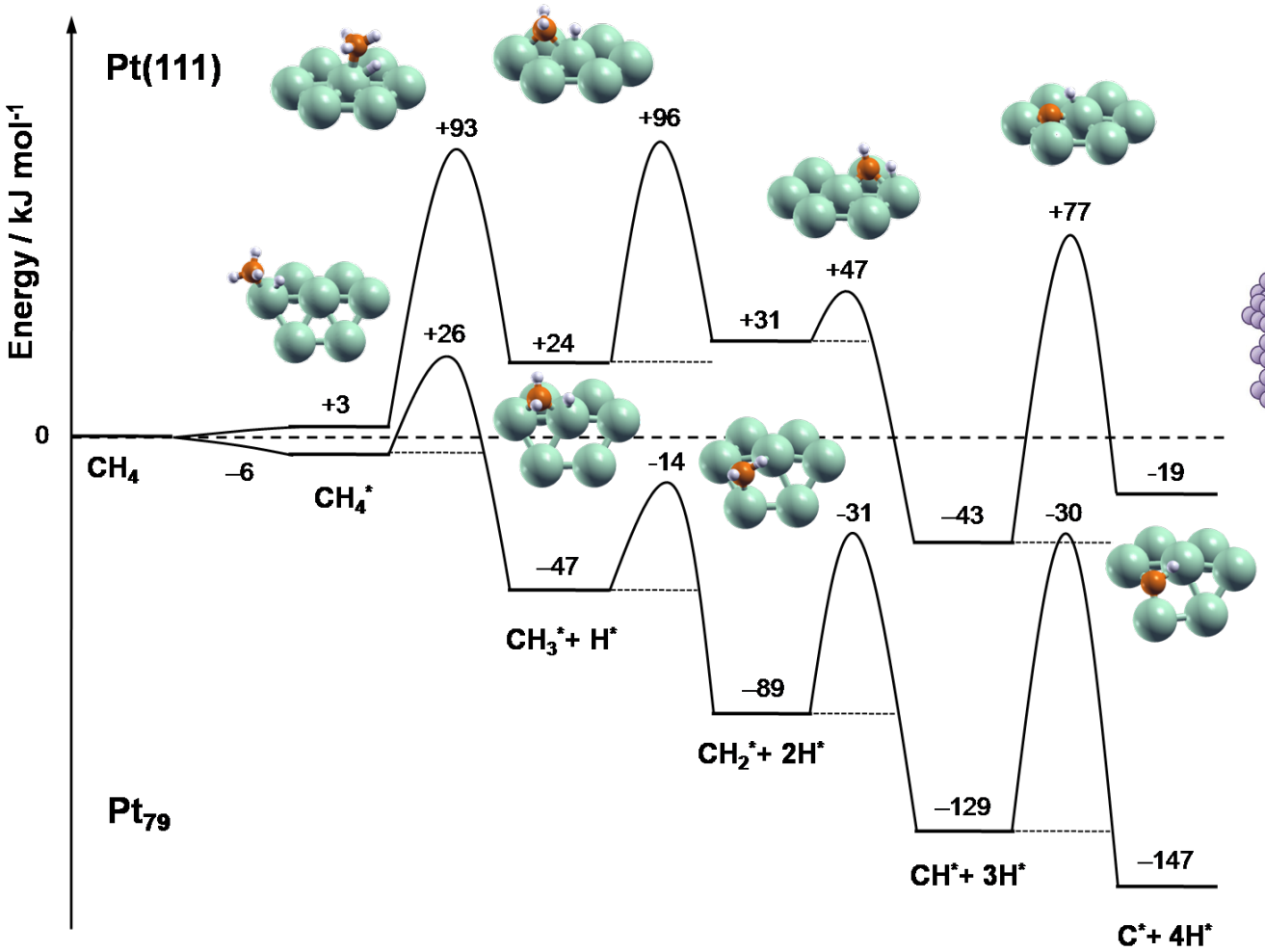
for investigation of

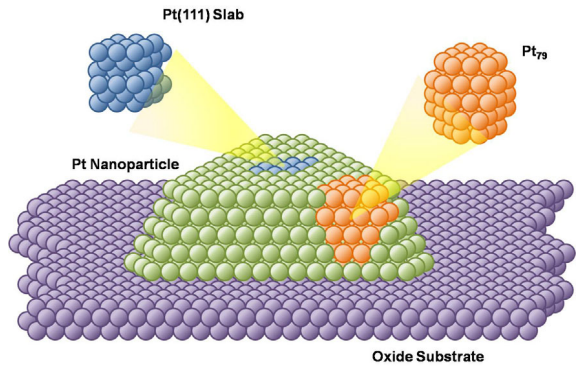
molecules, clusters, surfaces, and solids

with respect to

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

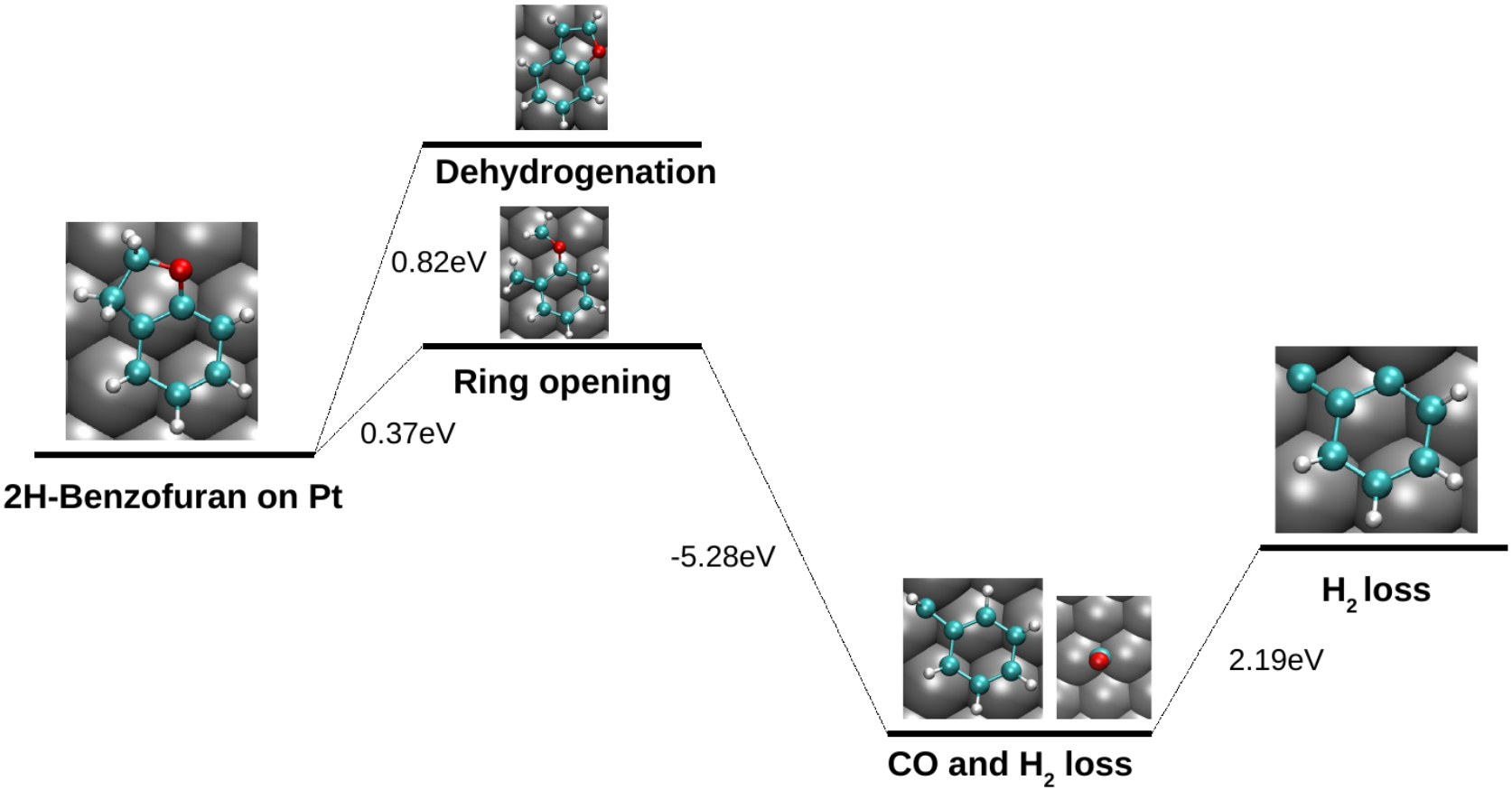
Methane decomposition on platinum surfaces and nanocrystallites



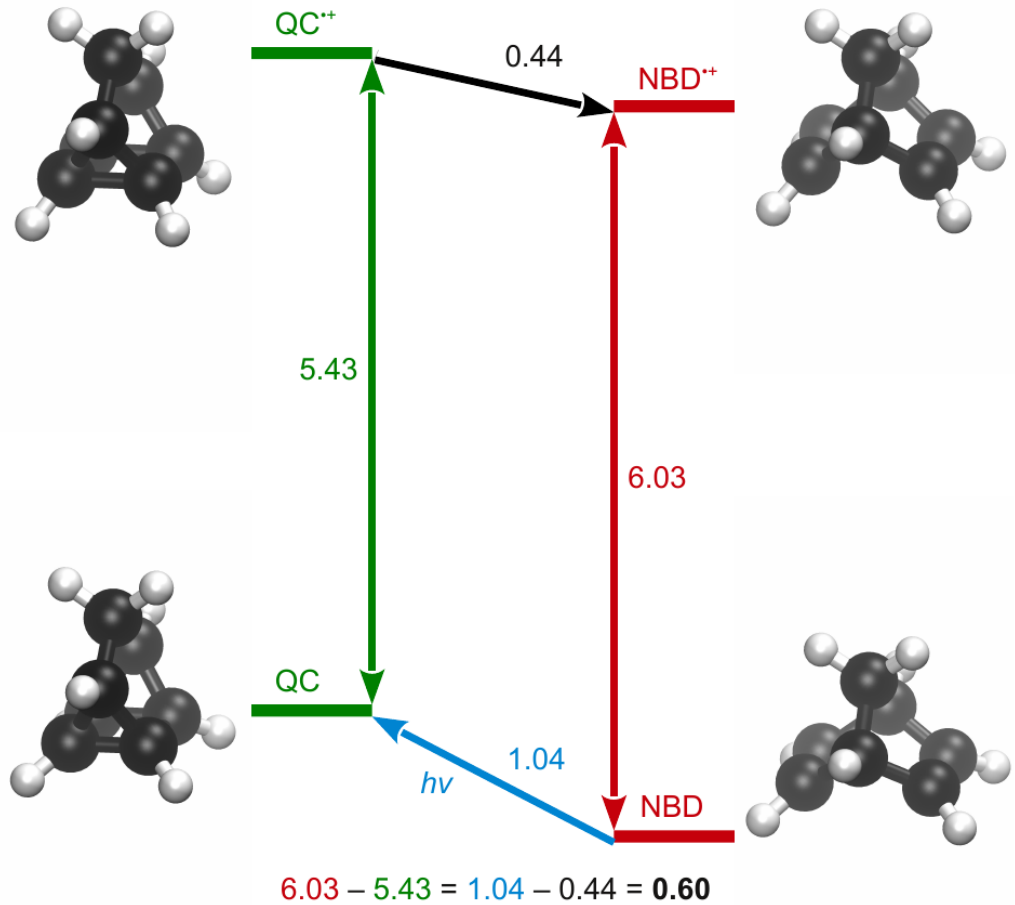


Collaboration with groups of J. Libuda and H.-P. Steinrück

Dehydrogenation of 2H-Benzofurane on Pt(111) surface



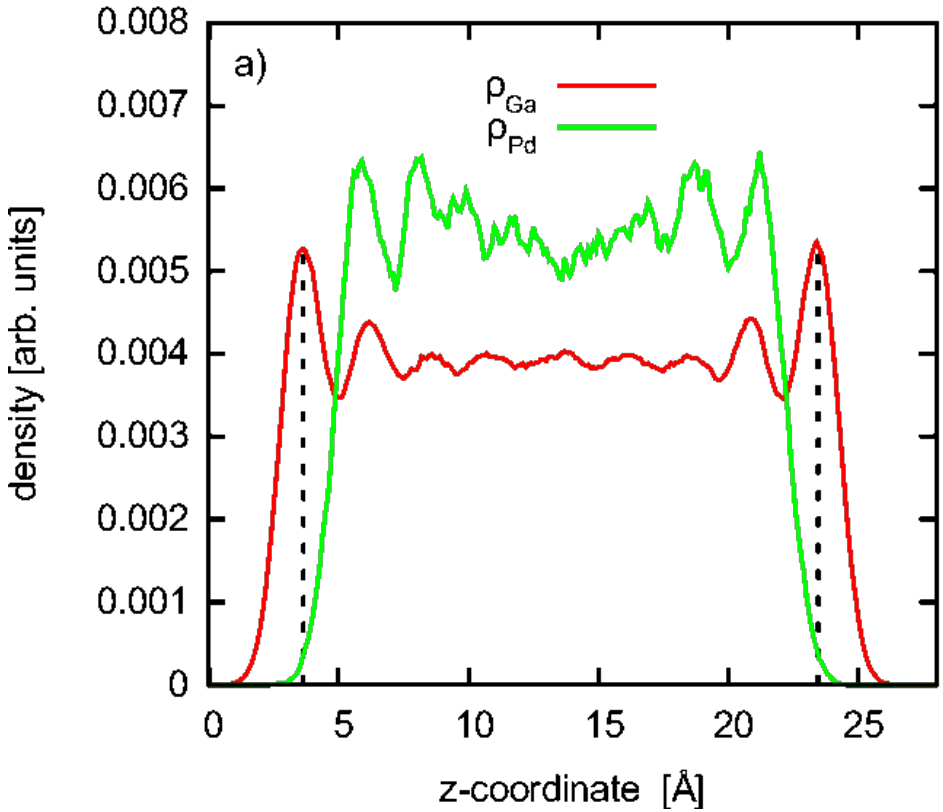
Collaboration with groups of C. Papp and P. Wasserscheid

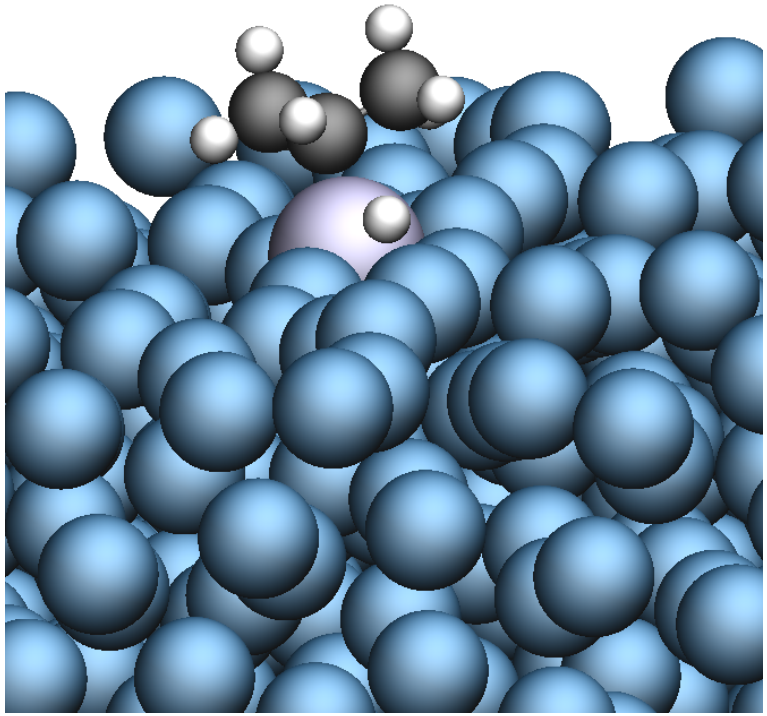


Collaboration with groups of A. Hirsch, J. Libuda, H.-P. Steinrück, and J. Bachmann

Catalysis with liquid metals

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

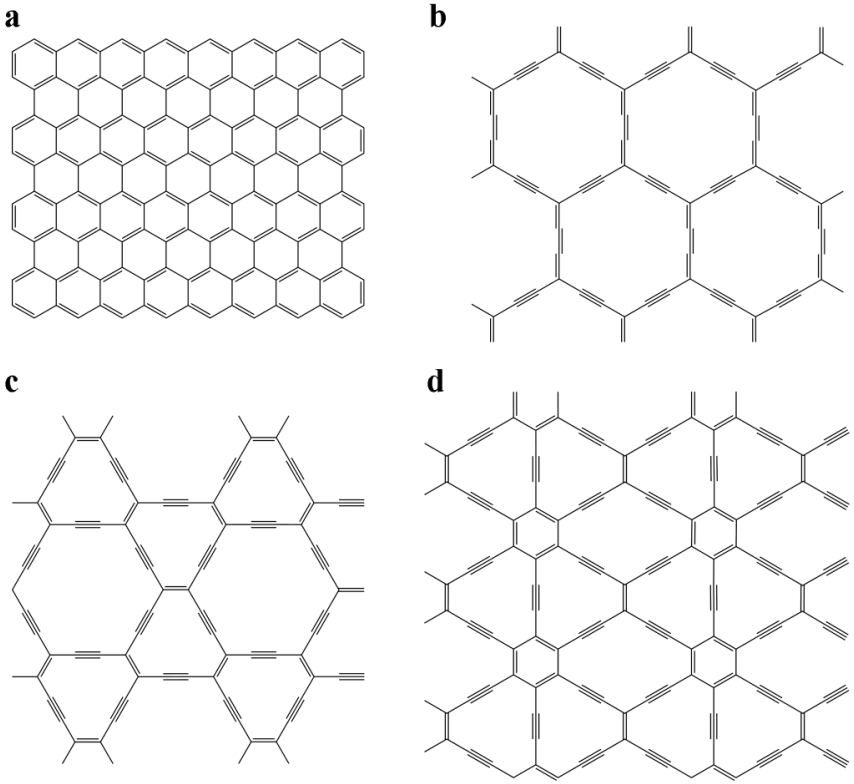


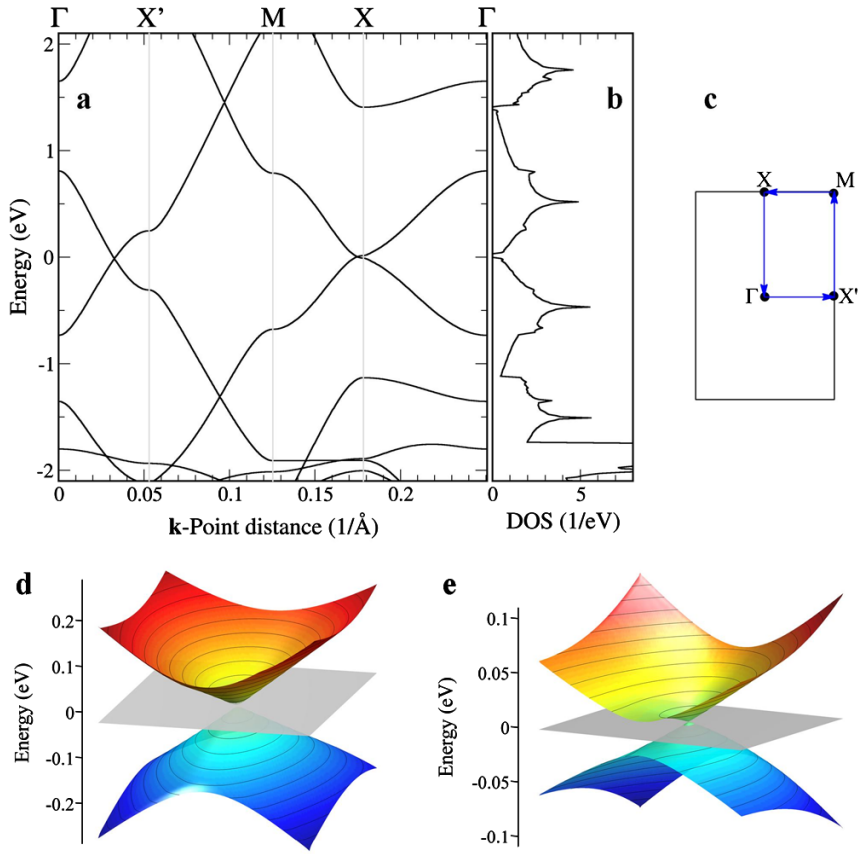


Within DFG collaborative research center 1452 "Catalysis at liquid interfaces"

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 Structure and energetics of novel carbon allotropes — Christian Neiß

2 New 2D materials — Joachim Paier

3 Organic molecules and ionic liquids on metal surfaces — Julien Steffen

4 Liquid organic hydrogen carriers — Christian Neiß

5 Liquid metal catalysis (ab-initio dynamics simulations) — Julien Steffen

6 Test of novel electronic structure methods — Steffen Fauser