Chemie und Materialwissenschaften mit dem Computer: Wellenfunktionen, Orbitale, und Elektronendichten in Spektroskopie, Katalyse und Synthese

Arbeitsgruppe Görling

Lehrstuhl für Theoretische Chemie

Arbeitsgebiet

Entwicklung und Anwendung von quantenchemischen Methoden

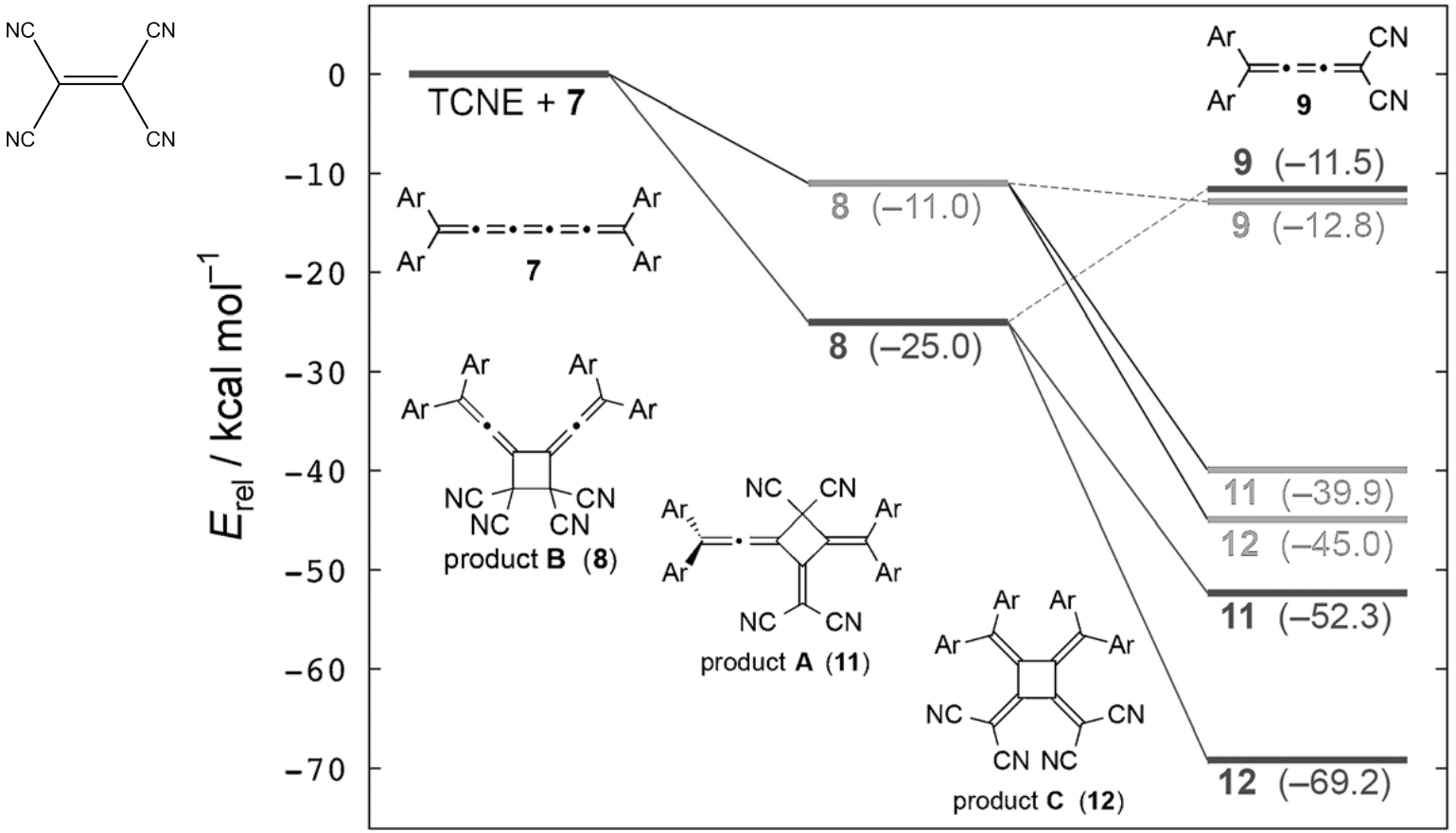
zur Untersuchung von

Molekülen, Clustern, Oberflächen und Festkörpern

hinsichtlich

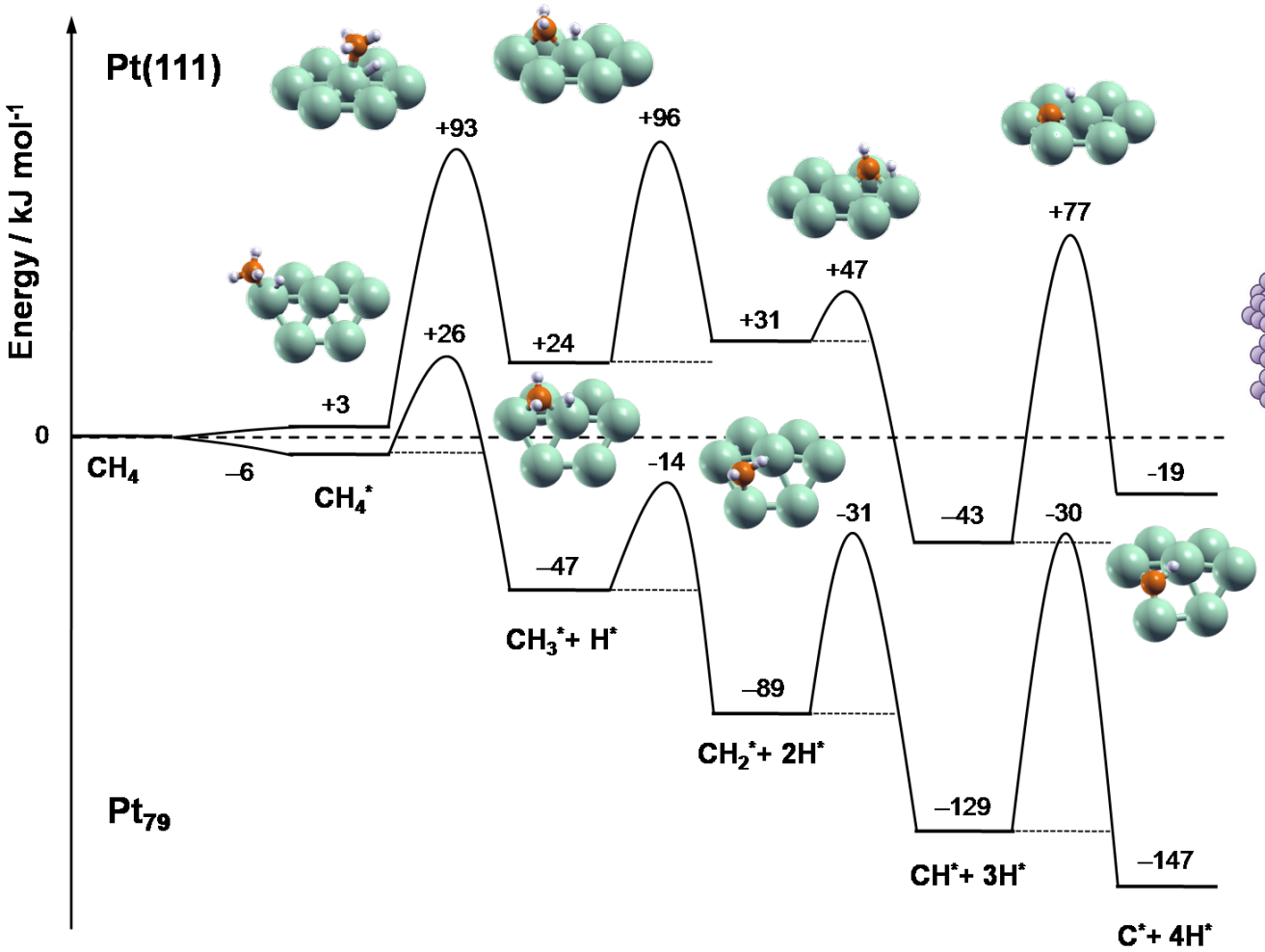
- Energetik und Struktur
- Reaktivität (Katalyse)
- Elektronischer Struktur (Orbitale, Bandstruktur, STM)
- Spektroskopie (UV/Vis, IR, NMR, nichtlinear optische Eigenschaften)

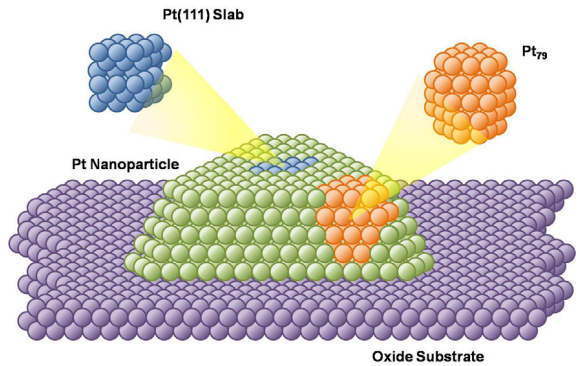
Unexpected Formation of a [4]Radialene and Dendralenes by Addition of Tetracyanoethylene to a Tetraaryl[5]cumulene



Collaboration with group of R. Tykwinski

Methane decomposition on platinum surfaces and nanocrystallites

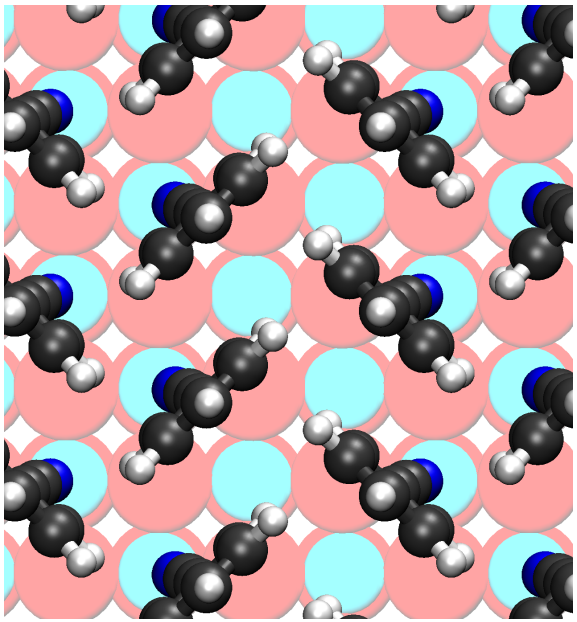
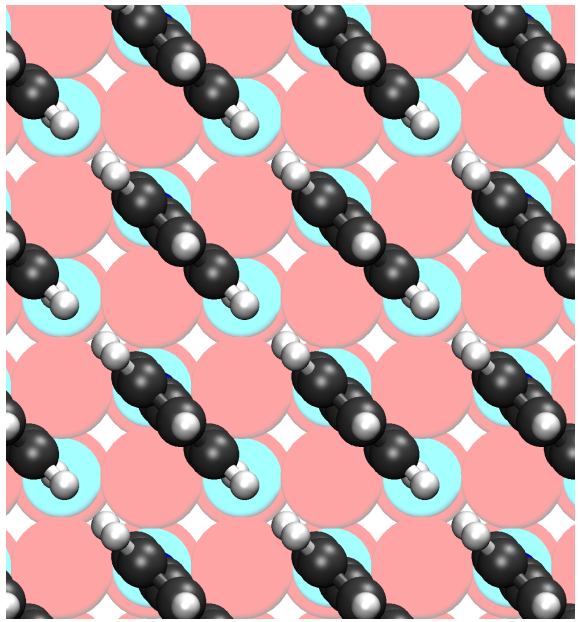
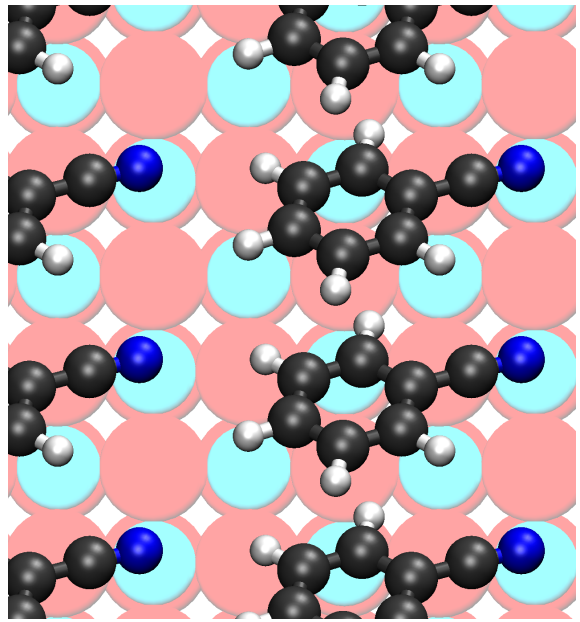




Collaboration with groups of J. Libuda and H.-P. Steinrück

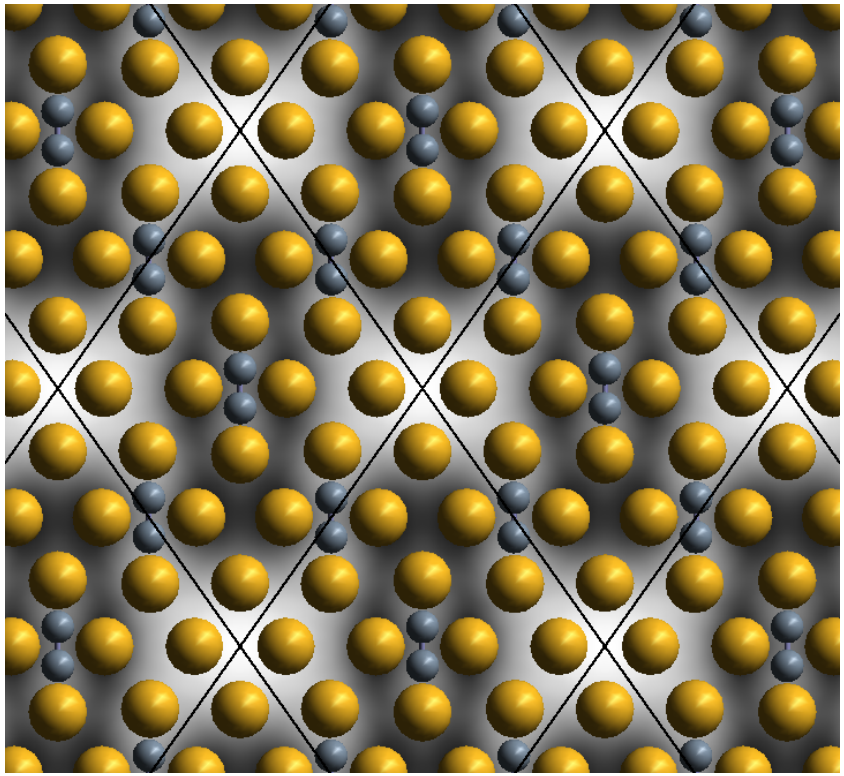
Adsorption of benzonitrile on MgO

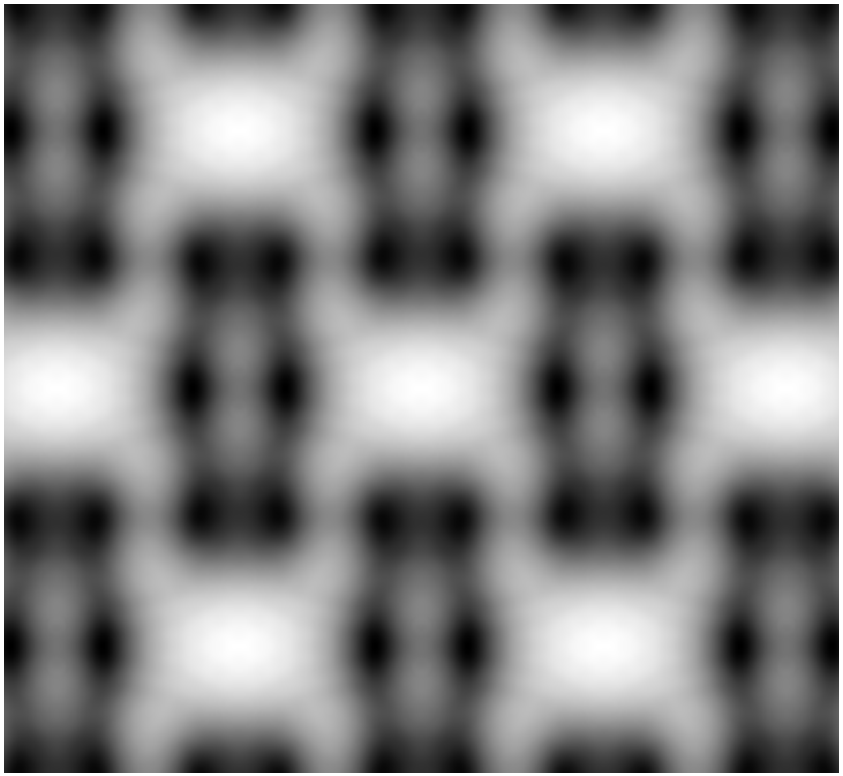
Self-organized layers of benzonitrile on MgO(100) depending on coverage

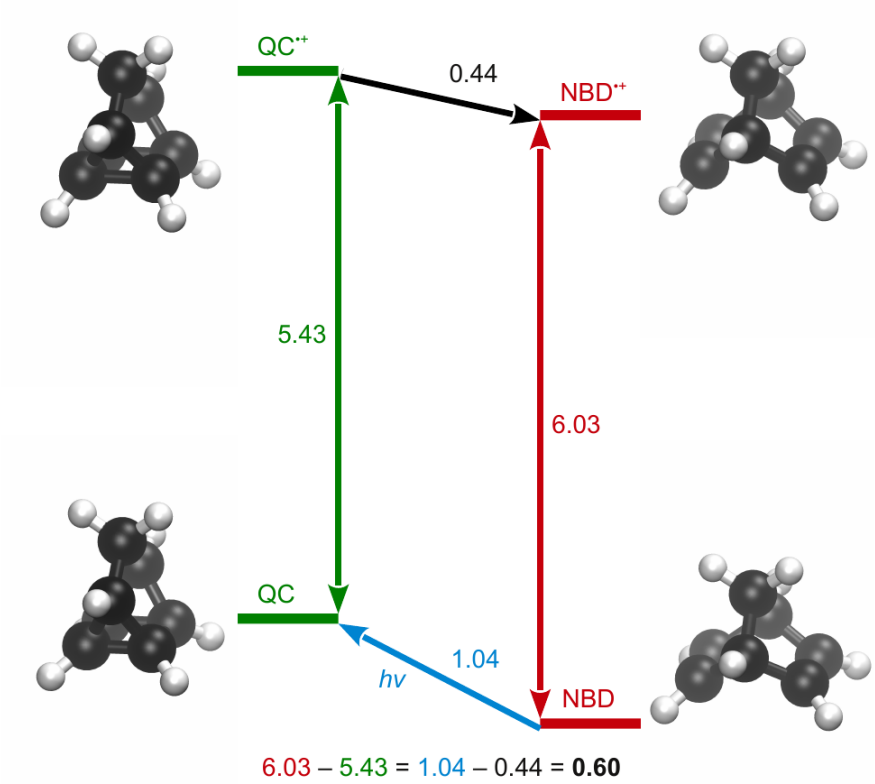
Collaboration with groups of J. Libuda, A. Schneider, S. Maier

Carbide-modified surfaces C/Mo(110)





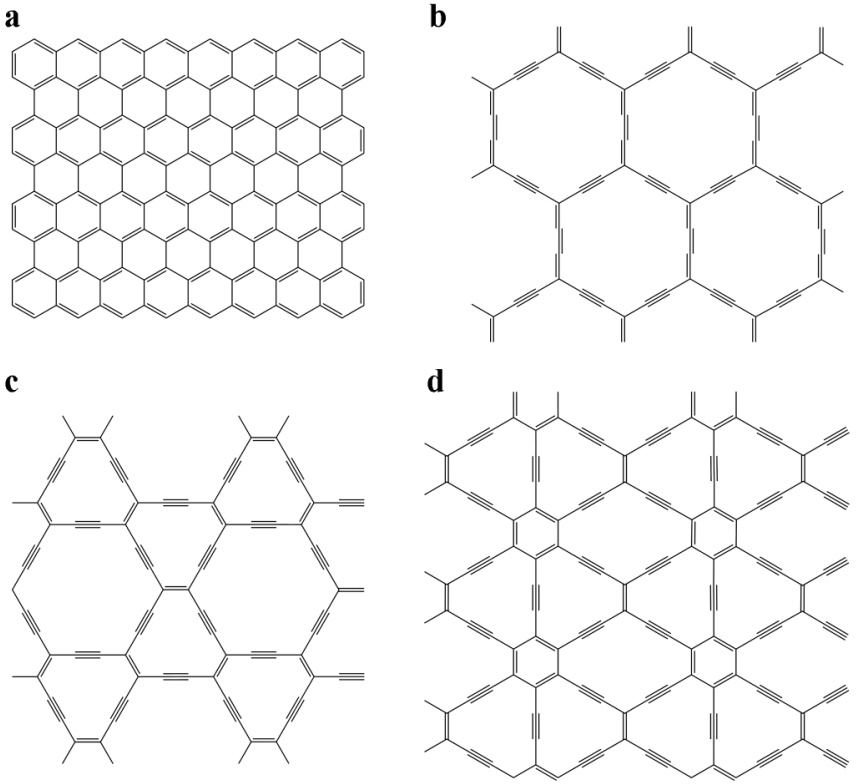
Collaboration with H.-P. Steinrück

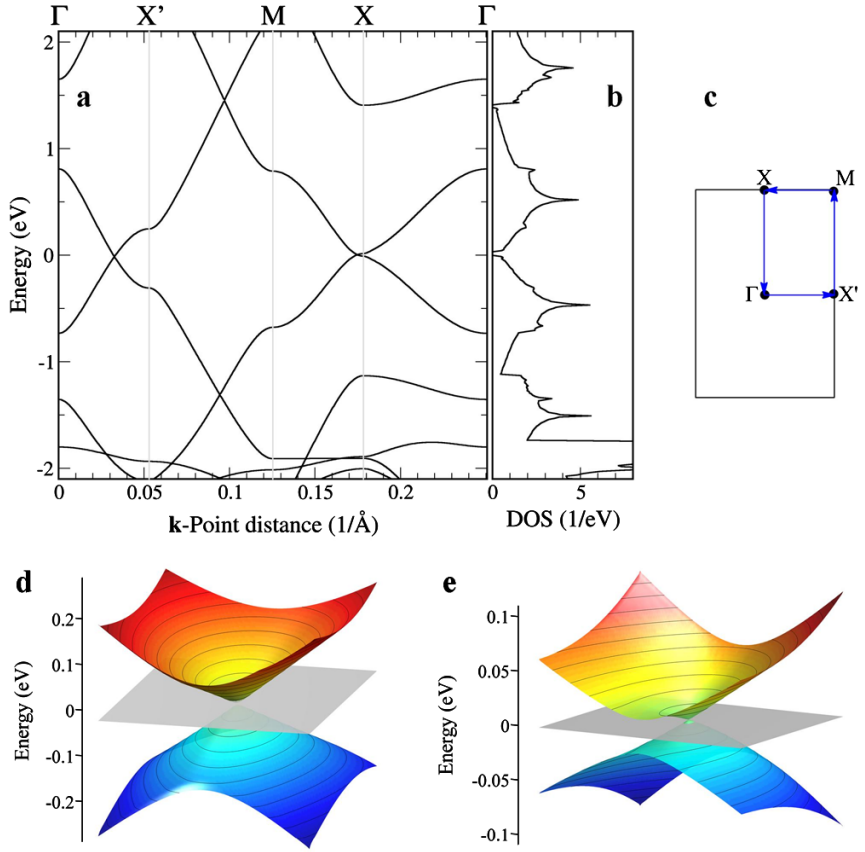


Collaboration with groups of A. Hirsch, J. Libuda, H.-P. Steinrück, and J. Bachmann

New carbon allotropes: graphynes

Alternatives to graphene with equally amazing electronic properties





Themen Bachelorarbeiten

1. Struktur und Energetik neuer Kohlenstoffallotrope — Himadri Soni
2. Neue 2D-Materialien, z. B. "blauer Phosphor" — Christian Neiß
3. Organische Moleküle auf Oxidoberflächen — Tibor Döpper
4. Materialien zur (elektro)chemischen Energiespeicherung — Christian Neiß / Tibor Döpper
5. Test neuer elektronischer Strukturmethoden — Daniel Schmidtel / Jannis Erhard