Institute for Multiscale Simulation

MSS

Master/Bachelor Thesis

Type

- Computational
- Experimental (optional)

Requirements

- Statistics and data analysis
- Basic knowledge of X-ray Scattering Theory (optional)
- Basic knowledge of Molecular Dynamics and Computer Graphics (optional)

QR code
zum pdf der Ausschreibung

For further information please contact:

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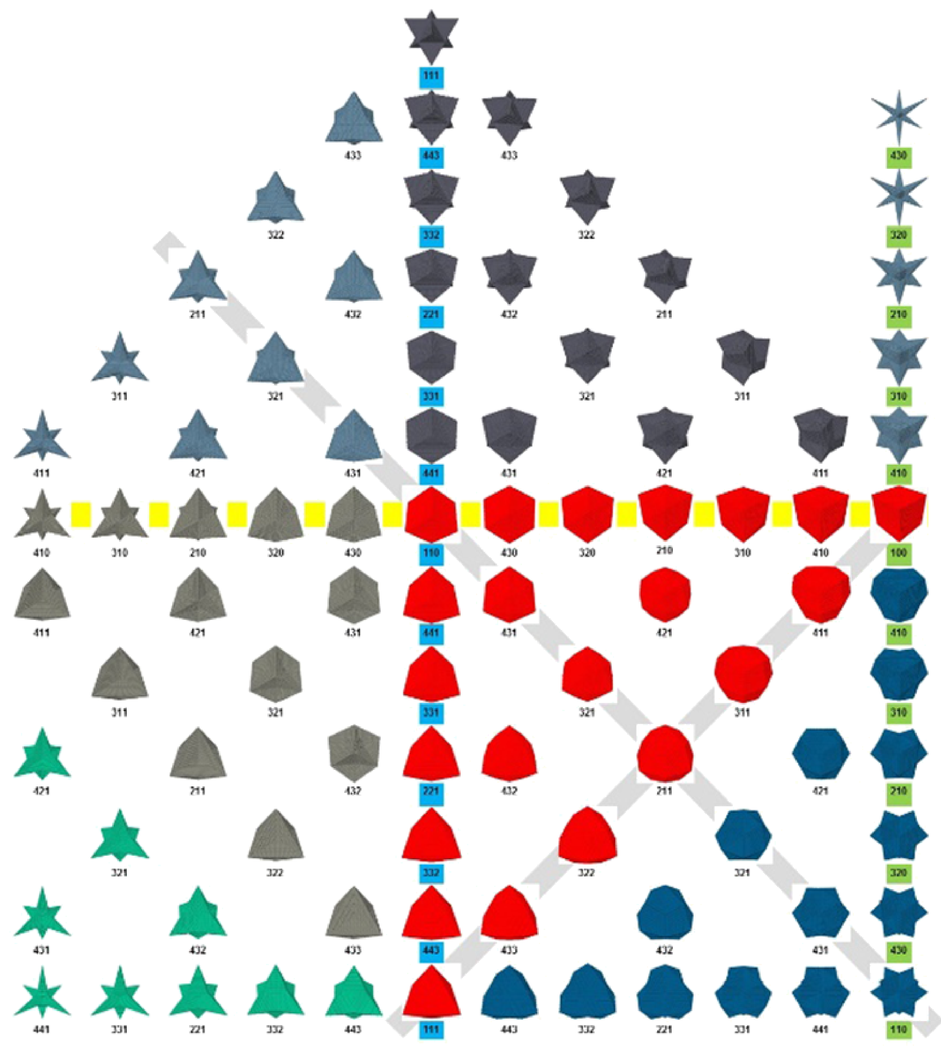
Chemical Activity of Shaped Nanocrystals

Background

Performance of metal nanoparticles for heterogeneous catalysis is influenced by the lattice structure deformation at the free surface of the nanocrystals. Control of size and shape allows to optimize such deformation thanks to the variation of the surface-to-volume ratio. Although such dependence is known for simple shapes (e.g., cube, octahedron, etc.), an systematic investigation of the shape influence is still missing.
Atomistic simulations of cubic Pd nanocrystals have been proven to provide results in full agreement with experimental evidence. Building on such validation a large scenario of polyhedral shaped Pd nanocrystals can be investigated. **Surface lattice strain can be systematically investigated as a function of the shape for constant volume or rather constant surface nanocrystals.**



Aim

- **Simulation of metal nanocrystals with polyehedral shapes**
- **Simulation of virtual powder X-ray diffraction experiments**
- **Study of the lattice distortion field**

- P. Scardi, et al., Phys. Rev. B 91 (2015) 155414
- Z. Chen, et al., Phys. Chem. C 121 (2017) 3