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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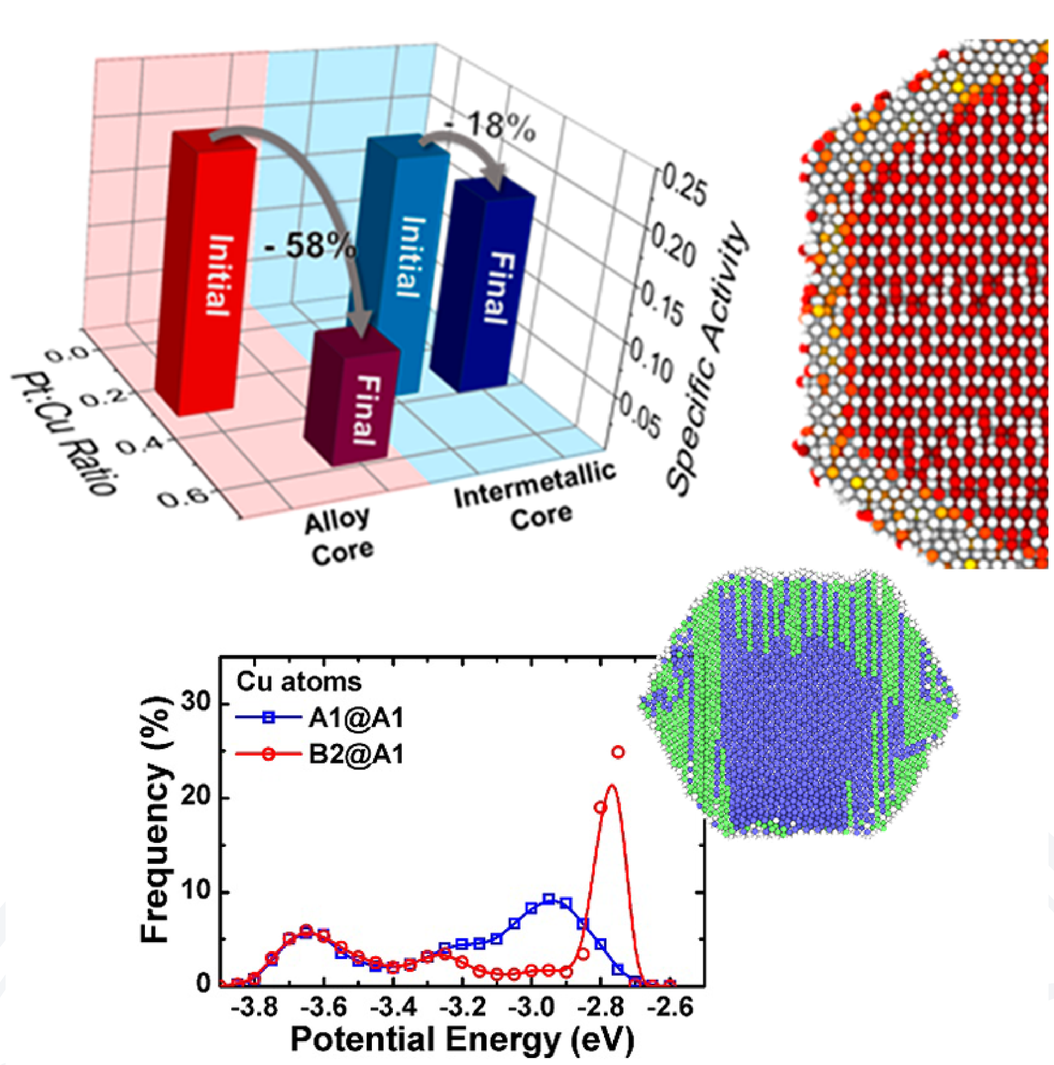
Phase Structure Transition in Core-Shell Nanocrystals

Background

Enhancement of chemical durability of multimtallic core-shell nanocatalysts can be achieved by mean of intermetallic core phase. However, synthesis of these order@disorder systems often exploits thermally activated phase structure transitions. We proved such enhancement for A1@A1 versus B2@A1 CuPd@CuPt nanocrystals via a combination of experiment and atomistic simulations.

CuAu alloys can also form ordered and disorderd crystal structure, namely A1 and L12. **Differently from the CuPd / CuPt mixtures, CuAu preserves the fcc cubic configuration.** Therefore, the interphase between the two phases is affected by a much smaller structure deformation, but in addition to the alloy phase two alternative L12 mixture are possible: Cu3Au and CuAu3.

Surface lattice strain can be systematically investigated as a function of the shape for constant volume or rather constant surface nanocrystals.



Aim

- **Simulation of Cu-Au core@shell nanocrystals**
- **Investigate the phase structure transition**
- **Verify the stability of ordered@disordered core@shell interface**

- J. T. Gamler, et al., ACS Nano 13 (2019) 4008