Within this project, hybrid interfaces between oxide surfaces (Fe₃O₄, TiO₂) and organic molecules (carboxylic acids, phosphonates, etc.) are investigated at the atomic length scale. The main goal is to obtain model systems which allow understanding, quantifying, and predicting material properties such as the thermodynamic stability. To this end, quantum-mechanics-based computational methods, mainly density functional theory (DFT), are employed to study the electronic and atomic structure of various interfaces. On top of DFT calculations, further methods like the cluster-expansion (CE) approach and Monte-Carlo (MC) simulations are used to scan configuration spaces exhaustively, to gain access to larger length scales, or to account for finite temperature effects. Key questions such as the structure, stability, and mechanical properties of the aforementioned hybrid interfaces including the influence of defects and co-adsorbates, or the shape of nanoparticles due to the presence of different ligands during their growth are addressed in close collaboration with the experimental projects A1, A6, A7 and other simulation projects like A5. This comprehensive approach allows us to gain fundamental knowledge on hybrid materials. A better understanding of their properties and phenomena at involved interfaces in the atomistic and nano domain will also facilitate the tailoring of properties of novel materials performed by various other projects on different hierarchical levels.

Key questions such as the structure, stability, and mechanical properties of the aforementioned hybrid interfaces including the influence of defects and co-adsorbates, or the shape of nanoparticles due to the presence of different ligands during their growth are addressed in close collaboration with the experimental projects A1, A6, A7 and other simulation projects like A5. This comprehensive approach allows us to gain fundamental knowledge on hybrid materials. A better understanding of their properties and phenomena at involved interfaces in the atomistic and nano domain will also facilitate the tailoring of properties of novel materials performed by various other projects on different hierarchical levels.

**Keywords**

hybrid interfaces  
adsorption  
surface science  
atomistic  
density functional theory  
organic molecules - oxide surfaces

**Publications**
