**GDCh-Kolloquium am Institut für Chemie neuer Materialien der**

**Universität Osnabrück**

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**Structure and reactivity of metal oxide surfaces and thin films –**

**Synergy of quantum chemistry and experiment**

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Thin film models that can be studied with surface science techniques are crucial for reducing the complexity of surface phenomena on solid metal oxides.

To gain atomistic insight into the metal oxide – water interface we study the interaction of water molecules with the MgO(001) surface for increasing loadings from isolated molecules to loadings beyond one monolayer. Issues addressed are the accuracy of modern quantum chemical ab initio methods beyond density functional theory, the sampling of configurations for higher coverages using genetic algorithms, the identification of adsorption structures using vibrational spectra, dissociative adsorption, and surface corrugation.

To address the question how reduced dimensionality changes structure and properties of solid oxides we consider ultrathin SiO2 films grown under ultra-high vacuum conditions on metal substrates, specifically crystalline films consisting of one or two layers of corner-sharing SiO4-tetrahedra and amorphous SiO2 phases that can be directly imaged in real space by scanning tunneling microscopy. Whereas doping (substitution) with Al is isomorphous (zeolite films), substitution of Si with Ti and Fe leads to new structure types.

Finally, the reactivity of CeO2, its role as catalyst support and the formation of oxygen defects are discussed.