a; post-doctoral fellowship at University of South Carolina (1998-2003).

Research

A project in my group that relates to CIMM deals with surface oxidation of high entropy alloys (HEA). The objective is to study the formation of different oxides on the multicomponent surface, particularly the competition among the oxide groups of the different atomic elements. Density Functional Theory (DFT) and Molecular Dynamics (MD)/DFT is used for these calculations. Individual O atoms, groups of O atoms and O layers are added on top of a HEA surface. DFT is first used to find an equilibrium geometry. The study then continues with MD/DFT that allows for chemical reactions to occur and the formation of oxide groups been predicted. Electronics density and Density of States allows to characterize chemical reactions leading to oxidation.