3RD VIENNA SCIENTIFIC CLUSTER USER WORKSHOP

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book of abstracts

HPC AS VALUABLE TOOL FOR THE INTERPRETATION OF EXPERIMENTAL SPECTROSCOPIC DATA IN COORDINATION CHEMISTRY

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Poster 5

Vibrational and optical spectroscopy are well known as very useful tool for the characterization of inorganic coordination compounds. With the program suite Gaussian09 rev.C using VSC-1 theoretical molecular spectroscopy is carried out and compared to experimental data in the field of small molecule organic chemistry and coordination chemistry. Within our contribution some of these applications of HPC in inorganic coordination chemistry are presented.

INITIO GUIDED DESIGN OF CORUNDUM TYPE (AL1-X-YCRXMY)2O3 THIN FILMS

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Poster 6

Sophisticated alloying concepts are of utmost importance for application oriented coating development in order to obtain specifically tailored and optimised material properties allowing for extended application ranges. Recent studies on borides, nitrides, or oxides have proven the effectiveness of combining first principle calculations with experimental developments in obtaining an atomistic-to-macroscopic understanding of high performance materials. In this work we describe the impact of several selected alloying elements (M) on the quasi-binary system of (Al1-xCrx)2O3 with focus on their capability to promote the desired corundum type phase. Based on ab initio calculated energies of formation for three different crystallographic structures (, cubic B1- like, and cubic) it was investigated if elements such as B, Si, Hf, Ta, or Y promote the formation of metastable cubic phases instead of the desired phase. The findings are compared with coatings synthesised by reactive cathodic arc evaporation. In the case of Fe alloying, for example, our predictions reveal no explicit impact on the phase stability sequence , B1-like, and , whereas experiments suggest an increased amount of phase fractions. Detailed analysis of the binding characteristics and structural defect sensibility provides an atomistic understanding of the sometimes observed discrepancy between calculations and experiments. This advanced approach allows for a knowledge-based development of high performance Al-Cr-based oxide coatings.