O 29: Oxides and insulators: Adsorption and reaction of small molecules – Poster

Time: Monday 18:00–20:00 Location: P2

O 29.1 Mon 18:00 P2

Impact of atomic oxygen on alumina surfaces investigated by molecular dynamics simulations — •Stephen Hocker, Hansjörg Lipp, and Johannes Roth — FMQ, University of Stuttgart, Germany

Oxygen atoms impinging on satellite surfaces in very low earth orbit (VLEO) transfer momentum and energy leading to material degradation as well as drag forces which result in orbital decay of the satellite. The first step in finding solutions to counteract significant drag is to gain understanding of the interaction of atomic oxygen (AO) with material surfaces. We investigate the angular and velocity distributions of reflected AO on crystalline and amorphous alumina surfaces using molecular dynamics simulations. Adsorption processes are evaluated and their influence on the surface structure and resulting changes regarding AO reflection is revealed. A strong dependence on the angle of incidence and the initial velocity is found. A high ratio of specular reflection can be obtained for grazing angles of incidence and hyperthermal initial velocities.

O 29.2 Mon 18:00 P2

First Principles investigation of the electronic properties and OER activity of (sub)stoichiometric WO_{3-x} (x =0.0, 0.1) — •Jeel Swami and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

Tungsten trioxide (WO_3) exhibits a rich sequence of temperature and defect-driven structural phase transitions. Using density functional theory (DFT) calculations with the SCAN0 (with and without a Hubbard U term) and HSE06 functionals, we explore the influence of oxygen defects on the electronic properties of WO_{3-x}. For substoichiometric Magnéli phase $WO_{2.9}$ our results show partial localization of charge at the interface exhibiting weak magnetisation and n-type conductivity. We further investigate the application of WO_3 as anode material for the oxygen evolution reaction. At the (001) facet we consider various surface terminations. Gibbs free energy plot reveal that *OOH formation is the potential determining step for WO_3(001) facet.

We acknowledge computation time at the MagnitUDE and AmplitUDE HPC systems at the University of Duisburg-Essen.

O 29.3 Mon 18:00 P2

Interaction of atomic Oxygen with Silica Surfaces — •Ahmad Kassem Arrak, Stephen Hocker, Hansjoerg Lipp, and Johannes Roth — FMQ, University of Stuttgart, Germany

In order to increase the lifetime of VLEO (very low earth orbit) satellites, the drag forces on the satellite and the degradation of the surface material must be reduced. Both arise mainly from atomic oxygen (AO) impinging on the satellite surfaces at hyperthermal velocities. We investigate the influence of AO impact on silica surfaces using molecular dynamics simulations (LAMMPS). A focus is on adsorption, reflection and chemical reactions. Three interaction potentials were used, one from Vashishta, a Tersoff potential and a PACE machine learning potential. We prepared three (001) surface structures of alpha silica differing by their surface layers. The oxygen impact simulations revealed that the interaction processes occurring at the surface depend strongly on the chemical composition of the surface layers. At the oxygen-rich surface the formation and desorption of O2 can be observed while reflection or adsorption of AO is favored at other surfaces.