

## O 53: Poster Session - Oxides and Insulators: Adsorption and Reaction of Small Molecules

Time: Tuesday 18:15–20:00

Location: P2/10G

O 53.1 Tue 18:15 P2/10G

**Investigation of Proton Conductivity in Yttria Stabilized Zirconia Thin Films by Electrochemical Impedance Spectroscopy** — •LARS-ERIK MAURER, ERDOGAN CELIK, and MATTHIAS T. ELM — Center for Materials Research, Gießen, Germany

Dense and porous yttria stabilized zirconia (YSZ) thin films were fabricated using pulsed laser deposition in order to investigate the influence of the layer thickness on the electrical and protonic transport properties under dry and wet atmospheres. For that purpose, electrochemical impedance spectroscopy was performed at different temperatures, oxygen partial pressures and relative humidities. Under dry atmospheres, the total conductivity of the thin films is dominated by oxygen vacancies and increases with increasing grain size due to the blocking behavior of the grain boundaries. At wet conditions, the total conductivity of the dense films is reduced which is attributed to an annihilation of the oxygen vacancies at the surface due to adsorbed water molecules. Only the porous layers exhibits a proton conductivity in wet atmosphere at low temperature and high relative humidity revealing the importance of the pore structure on the surface protonic conductivity of oxide materials.

O 53.2 Tue 18:15 P2/10G

**IRRAS study of CO adsorption on the calcite (10.4) surface** — WEIJIA WANG, •ALEXEI NEFEDOV, STEFAN HEISSLER, YUEMIN WANG, and CHRISTOF WOELL — Karlsruhe Institute of Technology, Institute of Functional Interfaces, Eggenstein-Leopoldshafen, Germany

The atomic structure of natural cleavage (10.4) calcite surface is a precondition to gain an understanding of its surface properties. To date, the atomic-level understanding of the structure is still under controversy. Therefore, in the present investigation, the (10.4) calcite surfaces were explored by the FTIR Spectroscopy with polarized infrared light in an ultrahigh vacuum (UHV) apparatus with the use of CO as a probe molecular. In order to achieve clean (10.4) calcite surface in UHV, dedicated devices (wobble stick, sample holder) are designed to perform the UHV cleavage. At low exposure, the adsorption of CO on the fresh cleaved (10.4) calcite surface at relatively low temperature of 62 K leads to a sharp negative C-O stretching band located at  $2175.8\text{ cm}^{-1}$  using the p-polarized infrared light. This band represents a coverage-induced frequency redshift trend before reaching to the saturated coverage. This observation provides the direct spectroscopic evidence that the cleaved calcite surface is a well-ordered surface.

O 53.3 Tue 18:15 P2/10G

**LEED Analysis of CO on NaCl(100) under Optical Excitation** — •LIAM SHELLING NETO, HANNES BÖCKMANN-CLEMENS, and CLAUS ROPERS — 4th Physical Institute - Solids and Nanostructures, University of Göttingen, Göttingen, Germany

Vibrational energy transfer between adsorbates and solid surfaces is of fundamental interest in surface science and has been explored in multiple contexts. In this regard, CO adsorbed on NaCl is a prominent model system, as its long vibrational lifetime allows for studying the energy flow between molecules via dipole-dipole interactions, which leads to the extreme concentration of vibrational energy at individual molecules. However, the structural modifications that accompany this process remain largely unknown and challenging to explore, for a lack

of a direct probe to observe their dynamics. Here, we use an ultrafast LEED setup to monitor the surface structure under optical excitation. The presented results constitute a preliminary step towards the understanding of the structural dynamics accompanying the vibrational energy transfer.

O 53.4 Tue 18:15 P2/10G

**Quantitative LEED studies of acetylene physisorbed on ionic surfaces – significance of electron scattering from hydrogen** — •JOCHEN VOGT — Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

$\text{C}_2\text{H}_2$  physisorption on ionic substrates is characterized by comparably soft interaction, leaving the internal structure of the molecules largely undistorted. On the KCl(100) surface, the first layer has  $(\sqrt{2} \times \sqrt{2})R45^\circ$  symmetry [1], while on the NaCl(100) surface,  $(3\sqrt{2} \times \sqrt{2})R45^\circ$  and even  $(7\sqrt{2} \times \sqrt{2})R45^\circ$  phases have been observed [2]. In principle, a complete structure determination of such systems is possible using LEED I(V) analysis [3,4]. Due to the weakness of electron scattering from hydrogen, this element was not included in a LEED study of  $\text{C}_2\text{H}_2$ -( $2 \times 2$ )/MgO(100) [4]. The contribution addresses the possible systematic error resulting from the neglect of hydrogen scattering in these systems. In the case of  $\text{C}_2\text{H}_2$ /KCl(100), calculated I(V) curves of the very weak superstructure spots are significantly affected by the neglect of hydrogen with respect to both intensity and the position of maxima, the latter implying notable changes of the Pendry R-factor. [1] A. L. Glebov et al., Phys. Rev. B61(2000), 14028 [2] S. Picaud et al., Phys. Rev. B57 (1998), 10090 [3] J. Vogt, H. Weiss, Phys. Rev. B77 (2008), 125415 [4] D. Ferry et al., Phys. Rev. Lett. 78 (1997), 4237

O 53.5 Tue 18:15 P2/10G

**Theoretical characterization of the surface and adsorption properties of water on titanium dioxide surfaces** — •HOLGER-DIETRICH SASSNICK<sup>1,2</sup>, SEBASTIEN GROH<sup>3</sup>, JOACHIM DZUBIELLA<sup>1,3</sup>, and VICTOR G. RUIZ<sup>1</sup> — <sup>1</sup>Research Group for Simulations of Energy Materials, Helmholtz-Zentrum Berlin, Berlin, Deutschland — <sup>2</sup>Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Deutschland — <sup>3</sup>Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Deutschland

Water splitting is a process for clean energy with promising technological applications to reduce environmental pollution and mitigate climate change. Rutile  $\text{TiO}_2(110)$  has become the prototypical oxide surface in surface science and its interaction with water a model system for the water-oxide interface. Even though extensive experimental and theoretical studies at the single-molecule level exist, the preferred adsorption state of water is still highly debated [U. Diebold, JCP 147, 040901 (2017)]. We present a thorough theoretical characterization of the surface and adsorption properties of water at the single-molecule level on the rutile (110) and the anatase (101) surfaces using density-functional theory including collective many-body effects in the dispersion interactions and a quantification of self-interaction error. In addition, we investigate coverage effects from the single-molecule to the monolayer regimes and quantify the dissociation barrier of a single water molecule. Our work aims to include all relevant effects at the electronic-structure level to quantify subtle changes on the water dissociation process and pave the way to more complex simulations of solid-liquid interfaces.