

O 29: Poster Session - Solid-liquid Interfaces: Structure, Spectroscopy

Time: Monday 18:15–20:00

Location: P1A

O 29.1 Mon 18:15 P1A

Enantioselective interactions of L- and D-alpha polyaniline molecules investigated by STM and STS — ●SHUYUAN XUE¹, NGUYEN THI NGOC HA¹, and CHRISTOPH TEGENKAMP^{1,2} — ¹TU Chemnitz, Germany — ²Leibniz Universität Hannover, Germany

The chiral induced spin selectivity (CISS) effect has been intensively investigated towards applications in molecular spintronics and spinselective processes in biology. The adsorption of a chiral molecules with a specific handedness affects the direction of the spin-polarization as well as magnetization of a surface [1]. For L alpha-helical polyaniline (PA) films on HOPG and Au(111) we found recently densely packed self-assembled monolayers. Thereby, interdigitation in between adjacent molecules favors also rotational order [2]. In this study we co-adsorbed L- and D-alpha polyaniline molecules from the liquid phase on HOPG and investigated the structure by scanning tunneling microscopy under ambient conditions. In contrast to L-alpha polyaniline molecules, the enantiometric mixture revealed a (2 x 1) structure. Apparently, the interdigitation takes place only along one crystallographic direction with one kind of molecules leading to phase separation of the enantiomers. [1] R. Naaman et al., *Chimia* 72, 394 (2018). [2] T.N.H. Nguyen et al. *J. Phys. Chem. C* 123, 612 (2019)

O 29.2 Mon 18:15 P1A

Ion adsorption and interface potentials of electrolyte solutions in contact with Au(111) including polarizability effects — VICTOR G. RUIZ¹, ZHUJIE LI², MATEJ KANDUČ³, and ●JOACHIM DZUBIELLA^{1,2} — ¹Research Group for Simulations of Energy Materials, Helmholtz-Zentrum Berlin — ²Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany — ³Department of Theoretical Physics, Jozef Stefan Institute, Ljubljana, Slovenia

Solid-liquid interfaces (SLI) are of growing interest to basic science and technology. SLI including gold (Au) have received much attention due to applications in catalysis and biotechnology. The need of including biomolecular and ionic species in the aqueous environment within atomistic simulations necessitates the accurate inclusion of charge and fluctuations effects of the liquids [Small 12, 2395 (2016)]. The formed interfaces are complex due to the interplay of van der Waals (vdW)

interactions, covalent bonds, and image-charge effects induced by the highly polarizable Au surface. Using a polarizable Lennard-Jones potential [I. Geadia, *et al.*, *Nat. Comm.* 9, 716 (2018)], we present molecular dynamics simulations of ionic adsorbates on Au(111) which include image-charge effects induced in the metal surface in a classical approximation. We present studies on the adsorption structures and interface electrostatic potentials of sodium chloride, sodium nitrophenolate, and sodium hexacyanoferrate salts, showing the influence which image-charge effects have on the interfacial microstructures and electrostatic properties.

O 29.3 Mon 18:15 P1A

Determining redox-dependent Cu-ligand chelating behaviour in a single metallo-protein — ●GIOVANNI GIUZIO¹, MASOUD BAGHERNEJAD^{1,2}, and KATRIN F. DOMKE¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Helmholtz-Institute, Münster, Germany

The copper metallo-protein azurin is a widely studied system in which ET is performed under physiological conditions by switching the oxidation state of the Cu center between +1 and +2.

In the presented project, we study individual azurin proteins bound to a Au(111) surface combining scanning tunneling microscopy and TERS under electrochemical conditions. In-air TER spectra show that the electronic, optical and vibrational properties of the azurin Cu center are preserved upon molecule conjugation with the Au surface. STM images prove that we TERS-probe individual proteins at a time.

Under EC conditions, we control the Au(111) potential which in turn regulates the oxidation state of the Cu center. The results show a potential-dependent behavior of the TER spectra. Comparing the S/N of in-air and in-liquid EC-experiment, a drastic signal reduction is observed under operando conditions. To improve the EC-TERS sensitivity, we use a spatial light modulator to optimize the laser-tip coupling, using either the focus size or the TER signal as a feedback. TERS potential-dynamic mapping of a single molecule switch and extracting structural information about the metallo-protein under switching conditions can be expected to provide unprecedented insights into ET transfer characteristics in biomolecular switches.