

O 57: Poster Wednesday: Electronic Structure

Time: Wednesday 18:00–20:00

Location: P4

O 57.1 Wed 18:00 P4

Josephson effect in the two-band superconductor Niobium Diselenide — ●XIANZHE ZENG¹, HAONAN HUANG¹, SUJOY KARAN¹, KLAUS KERN^{1,2}, and CHRISTIAN AST¹ — ¹Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — ²Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Niobium Diselenide is a two-dimensional (2D) van der Waals s-wave superconductor that can be described by a two-band model. The Josephson effect between Niobium Diselenide and another known BCS superconductor is non-trivial since it involves Copper pair tunneling of two bands with different order parameters. Here, we measure quasi-particle tunneling as well as the Josephson current between a clean superconducting Niobium Diselenide surface and a superconducting Vanadium tip using low-temperature scanning tunneling microscopy and spectroscopy. We analyze our results with the McMillan formula for a two-band superconductor. Our observations present a first step towards understanding more complicated scenarios, such as the predicted p-wave triplet superconductivity in Chromium Tribromide islands on Niobium Diselenide.

O 57.2 Wed 18:00 P4

Bulk Ion Conductivity and Near Surface Composition of Ionic Liquid and Zwitterionic Salt Based Electrolytes for Lithium Battery Applications — ●FABIAN ULLMANN, JOEL TAYO, ANNA DIMITROVA, and STEFAN KRISCHOK — Institut für Mikro und Nanotechnologien, Institut für Physik, TU Ilmenau

In this contribution we focus on the bulk conductivity and the near surface composition of several tertiary electrolytes which consist of Ionic Liquid (IL), Zwitterionic salt (ZwS) and lithium salt. Two ILs and ZwSs are chosen: IL: 1-ethyl-3-methylimidazolium bis-(trifluoromethylsulfonyl)imide - [EMIm][Tf2N] and 1-butyl-1-methylpyrrolidinium bis-(trifluoromethylsulfonyl)imide - [BMP][Tf2N]; ZwS: 3-(3-methylimidazolium-1-yl)Propane-1-sulfonate and 3-(3-vinylimidazolium-1-yl)Propane-1-sulfonate. As lithium precursor - bis(trifluoromethylsulfonyl)imide - Li[Tf2N] was used. Different Li[Tf2N]/ZwS ratios are considered and studied. Electrochemical Impedance Spectroscopy (EIS) enables us to determine the ion conductivity of the electrolytes. The results reveal that the presence of ZwSs enhances the ion conductivity, although they itself are not ion conductive. Further, by using X-Ray Photoelectron Spectroscopy (XPS) we analyze the near surface chemical composition at UHV-conditions. The XPS analysis displays a cation/anion/ZwS distribution as depended on the concentration of Li[Tf2N] and the type of IL and ZwS used. The spectroscopic results revealed solute-solvent interactions which modify the ion mobility.

O 57.3 Wed 18:00 P4

Line shape analysis of the resonant eigenstates in a quantum corral by means of tunneling spectroscopy and non contact AFM — ●MARCO WEISS, MICHAEL ROESSNER, FABIAN STILP, and FRANZ J. GIESSIBL — Institute of Experimental and Applied Physics, University of Regensburg, Germany

Back in 1993 Crommie et al. [1] arranged 48 Fe adatoms on a Cu(111) surface in a circle with a diameter of 14.26 nm. This quantum corral confines surface electrons in a circular potential well. Past investigations with scanning tunneling microscopy revealed energetically discrete eigenstates that spatially appear as Bessel functions. But these studies on the Fe quantum corral showed unwanted movement of the corral walls during spectroscopic measurements. [1]

Instead of Fe, we used CO molecules to provide the corral with more stable walls. This permitted us to access a larger voltage window and allowed for a detailed line shape analysis of the corrals eigenenergy levels. Surprisingly, we discovered a large Gaussian broadening of the eigenstates.

We also acquired nc-AFM data of the corral. As we have previously done, we determined the occupation of electronic states that cross the Fermi level [2]. Similar to our previous work, we observed that the presence of the probe tip shifts the energy of the electronic states under study. In this work, we show that we can also use the AFM data to estimate the lifetime (i.e. the spectral width) of these states.

[1] M. F. Crommie et al., Science 262, 218-220 (1993)

[2] F. Stilp et al., Science 372, 1196-1200 (2021)

O 57.4 Wed 18:00 P4

Interaction between an artificial and a natural atom — ●FABIAN STILP, MARCO WEISS, and FRANZ J. GIESSIBL — University of Regensburg, Regensburg, Germany

The surface state of Cu (111), a quasi-2-dimensional electron gas, is trapped to a small surface area of about 15 x 15 nm² by placing 48 CO-molecules in a circular shape on the surface via atomic manipulation. By doing so, one creates a quantum corral with discrete electronic states forming an artificial atom. This structure can be described reasonably well by an infinitely high circular potential well leading to corral states with Bessel-type radial functions and an angular momentum normal to the surface. To investigate the interaction between this artificial atom and a natural atom we bring Fe atoms inside the corral and measure the response of the corral states.

Thanks to the large size, one can study the structure of the wave functions within that artificial atom by nc-AFM showing an angular dependence of the corral states after placing the atoms inside the corral. This change of the wave functions leads to an energy shift of a few meV confirmed by tunneling spectroscopy measurements. By investigating the change of the wave functions and the energies of the corral states when placing the adatom inside, one can draw conclusion about the interaction between this artificial atom and a natural atom. Here we expand the interpretation of the adatom acting repulsively on the corral states as stated by Stilp et al. [1].

[1] F. Stilp, A. Berezuk, J. Berwanger, N. Mundigl, K. Richter, F.J. Giessibl, Science 372, 1196-1200 (2021)

O 57.5 Wed 18:00 P4

Spontaneous Charge Localization on Polar Surfaces — ●MICHELE RETICCIOLI¹, ZHICHANG WANG^{2,3}, ZDENEK JAKUB², IGOR SOKOLOVIC², MATTHIAS MEIER^{1,2}, GARETH S. PARKINSON², MICHAEL SCHMID², DOMINIK WRANA⁴, LYNN A. BOATNER⁵, ULRIKE DIEBOLD², MARTIN SETVIN^{2,4}, and CESARE FRANCHINI^{1,6} — ¹Faculty of Physics and Center for Computational Materials Science, University of Vienna, Austria — ²Institute of Applied Physics, TU Wien, Vienna, Austria — ³State Key Laboratory for Physical Chemistry of Solid Surfaces, Xiamen University, China — ⁴Department of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — ⁵Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, USA — ⁶University of Bologna, Italy

Excess charge on polar surfaces of ionic compounds is commonly described by the two-dimensional electron gas (2DEG) model, a homogeneous distribution of charge confined in a few atomic layers. Conversely, our density functional theory calculations and scanning-probe microscopy measurements on KTaO₃(001) show spontaneous localization of the excess charge in the form of polarons, bipolarons and charge density waves. These electronic reconstructions form on the defect-free surface, and alter the material properties and functionalities to different degrees. Controlling the degree of charge ordering could be of great benefit for a wide range of applications: in our study, we analyze the impact on the surface reactivity by considering the interaction with CO molecules.

O 57.6 Wed 18:00 P4

Evolution of Property and Bonding Maps — ●CARL-FRIEDRICH SCHÖN and MATTHIAS WUTTIG — RWTH Aachen University, Aachen, Germany

Since picking up the first tool, it has been the goal of mankind to create materials that best suit human needs. While for the longest time any development in this field was driven by an empirical approach, modern means of physics and chemistry gave rise to the concept of material and property maps based on chemical bonding. We have composed a database of elemental and binary compounds. For all compounds, the corresponding values of a set of properties were included, containing the conductivity, the Born Effective Charge, the Effective Coordination Number (ECoN) and the Bandgap, the melting point, the density and the atomic density. A Gaussian mixture algorithm was utilized to separate the compounds in the database into n clusters. With the number of allowed clusters set to 4, the algorithm nicely separates materials

which employ metallic, ionic and covalent bonding. This implies that properties can be used to distinguish bonding mechanisms. Interestingly, a fourth class of materials is identified, characterized by a property portfolio neither found in metals, or materials employing ionic or covalent bonding. This is further support for the concept of metavalent bonding, a novel bond type characterized by the competition between localization and delocalization. This classification provides a close link between chemical bonding mechanisms and properties enabling novel routes to material's design with material maps.

O 57.7 Wed 18:00 P4

A theoretical investigation into gallic acid pyrolysis — ●JAKOB KRAUS and JENS KORTUS — Institute of Theoretical Physics, TU

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Thermodynamical and kinetic information on the first two steps of gallic acid pyrolysis is calculated based on density functional theory and quantum chemistry. For the kinetics, transition states are identified with the help of the climbing image nudged elastic band method. Both reactions exhibit two transition states. One of them is related to the rotation of OH groups, and the other one is related to the breaking and forming of bonds. The gallic acid pyrolysis as a whole is judged to be endothermic, and it changes from endergonic to exergonic between 500 K and 750 K. The second reaction step, the dehydrogenation of pyrogallol, is identified as the limiting step of gallic acid pyrolysis, with reaction rate constants below 1 s^{-1} for temperatures below 1250 K.