O 9: Semiconductor Substrates I: Adsorption of Small Molecules, Metallic Nanowires, Overlayers

Time: Monday 10:30–12:15 Location: MA 144

O 9.1 Mon 10:30 MA 144

Bayesian and Multi-Objective Optimization for Sensor Technologies — •Ransell D'Souza[1], Shuja Malik[2], Fatima Annanouch[2], Eduard Valero[2], and Milica Todorović[1] — [1]University of Turku, Turku, Finland — [2]Universitat Rovira i Virgili

Sensors, a device that can detect toxic and combustible gasses, play a crucial role in identifying potentially hazardous gas leaks. Sensors typically function by employing inorganic substrates that respond to the adsorption of target molecules. To design selective and sensitive sensors, density functional theory studies should explore the interplay between adsorption energies, charge transfer, recovery time, and sensor response during interactions between toxic targets and the substrate.

While conventional computational approaches have focused on individual material properties, we need to balance different considerations of these properties for a truly predictive sensor design. This presents a multi-objective optimization problem, which can be effectively addressed using Bayesian Optimization (BO)-based machine learning techniques.

In this study, we employ multi-objective BO techniques to investigate the stable adsorbate structures of NH_3 on WS_2. We identify optimal tradeoffs between energetically stable structures and optimal response functions (Pareto optimal solutions) for the rational design of new sensors. Our resistivity and sensor response functions agree with experimental data, validating active learning's success in gas sensor material optimization.

O 9.2 Mon 10:45 MA 144

N-Heterocyclic Olefins on a Silicon Surface — •Martin Franz[1], Mowpriya Das[2], Conor Hogan[3,4], Robert Zielinski[1], Milan Kubicki[1], Maximilian Koy[2], Canan Kosbab[1], Simone Brozzesi[4], Ankita Das[2], Mike Thomas Nehring[1], Viktoria Balfanz[1], Juls Brühne[1], Mario Dähne[1], Norbert Esser[1,5], and Frank Glorius[2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Westfälische Wilhelms-Universität Münster, Organisch-Chemisches Institut, Münster, Germany — [3]Istituto di Struttura della Materia-CNR (ISM-CNR), Rome, Italy — [4]Università di Roma "Tor Vergata", Dipartimento di Fisica, Rome, Italy — [5]Leibniz-Institut für Analytische Wissenschaften "ISAS e.V.", Berlin, Germany

N-Heterocyclic carbenes are known to be excellent ligands for surface modification, and recently also the formation of ordered monolayers on silicon has been reported [1]. In contrast, surface adsorption of their close relatives, the N-heterocyclic olefins (NHOs), has not been studied yet. Here, a combined scanning tunneling microscopy, X-ray photoelectron spectroscopy, and density functional theory study of NHOs on silicon is presented. We find that the two studied NHOs bind covalently with ylidic character to the silicon adatoms of the substrate and exhibit good thermal stability. The adsorption geometry is found to depend on the N-substituents and strongly influences the quality and properties of the obtained monolayers.

[1] M. Franz et al., Nat. Chem. **13**, 828-835 (2021).

[2] M. Das et al., Angew. Chem. Int. Ed. **2023**, e202314663.

O 9.3 Mon 11:00 MA 144

Adsorption of cysteine on the surface of TiO2 — •Miguel Blanco Garcia[1], Mona Kohantorabi[1], Andreas Stierle[1,2], and Heshmat Noei[1,2] — [1]Centre for X-ray and Nanoscience (CXNS), Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Ham-burg, Germany — [2]Fachbereich Physik Universität Hamburg, Jungiusstr. 9-11, D-20355, Hamburg, Germany

Titanium oxide stand as a promising material for the inactivation of the viruses under light irradiation [1]. Our investigation centers on the most abundant amino acid within the spike proteins of SARS-CoV-2, cysteine [2], exploring its adsorption behavior on the surface of TiO2 under ultra-high vacuum (UHV) and aqueous conditions. Employing X-ray photoelectron spectroscopy, we observe UV light induces desorption of the cysteine molecule as well as its mineralization. Fourier-Transform Infrared Reflection Absorption Spectroscopy (FT-IRRAS) sheds light on the preferred binding modes and molecular arrangement of the cysteine during adsorption on TiO2. In addition, FT-IRRAS elucidates which bonds are influenced by UV treatment and unveils the molecular breakdown process. Furthermore, we monitored the adsorption of cysteine with TiO2 in an aqueous solution using Grazing-Incidence Small-Angle X-ray Scattering (GISAXS) at DESY P03 beam line which provides further information on the adsorption geometry and self-assembly of the cysteine amino acid TiO2 surfaces. [2] Kohantorabi, et al., ACS Appl. Mater. Interface., 15 (2023) 8770-8782. [3] Wang D, et al., Nano today 40 (2021) 101243.

O 9.4 Mon 11:15 MA 144

The impact of adatom adsorption on the interfacial structure of InP(001) — •Vibhav Yadav[1,2], Margot Guidat[1,2], Mario Löw[2], Jognmin Kim[1,2], Holger Euchner[1], and Matthias May[1,2] — [1]Institute of Physical and Theoretical Chemistry, Universität Tübingen, — [2]Institute of Theoretical Chemistry, Universität Ulm, Germany

Controlling the electrochemical interface of III-V semiconductors such as InP is of great relevance for hydrogen production in Photoelectrochemical water-splitting devices [1]. Here, reducing corrosion, while at the same time maintaining efficient charge transfer, remains challenging and requires an atomistic understanding of the InP(001) surface in an electrochemical environment. While InP(001) is known to exhibit different surface reconstructions, depending on the exact synthesis conditions, the presence of oxygen strongly affects the surface structure.

In this work, we apply Density Functional Theory to investigate the thermodynamic stability of the different reconstructions pertaining to adatom exposure such as oxygen, finally resulting in an extended surface phase diagram. Furthermore, we show that combining computational and experimental Reflection Anisotropy Spectroscopy has the potential to provide a better understanding of InP surfaces/interfaces and their (electronic) structure under operation conditions[2].

[1] : May MM; Lewerenz HJ; Lackner D; Dimroth F; Hannappel T. In: Nat Commun 6.1 (Sept. 15, 2015), p. 8286

[2] :Löw, M.; Guidat, M.; Kim, J.; May, M. M. RSC Adv. 2022, 12 (50), 32756*32764

O 9.5 Mon 11:30 MA 144

Realizing strictly one dimensional behavior in arrays of atomic wires on semiconducting substrate emerging from dispersive two dimensional system — Keshab Sony and •Anas Abdelwahab — Leibniz Universität Hannover, Hanover, Germany

We studied single and two Su-Shreiffer-Heeger wires on simple cubic semiconducting substrate. The wire-wire coupling is either perpendicular or diagonal hopping respecting the particle-hole and time-reversal symmetries. The hybridization to substrate renormalizes the model parameters of the wires towards the hopping parameter of the substrate without changing the basic nature of perpendicular or diagonal coupling and it can mediate effective perpendicular hopping but not diagonal hopping in the absence of direct wire-wire coupling. This justifies the investigation of multi uniform tight binding wires with perpendicular or diagonal hopping parameters while neglecting the substrate. Perpendicularly coupled uniform wires reveal anisotropic two dimensional band dispersion. Diagonally coupled uniform wires reveal strictly one dimensional bands parallel to the wires direction if the intra-wire hopping parameter is larger than twice the diagonal hopping parameter despite strong dispersion perpendicular to the wires. Otherwise, they reveal strictly one dimensional bands parallel and perpendicular to the wires direction simultaneously. We established the possibility of realizing strictly one dimensional properties emerging from dispersive two dimensional system if time-reversal and particle-hole symmetries are respected. This can facilitate the debate on one dimensional behavior of the Au/Ge(001) surface reconstruction.

O 9.6 Mon 11:45 MA 144

Diffusive mass transport of Pb on Si(111) (7x7) — •Felix Hartmann[1], Paul P. Schmidt[1], Regina Hoffmann-Vogel[1], Ralf Metzler[1,3], and Janet Anders[1,2] — [1]Institute of Physics and Astronomy, University of Potsdam, 14467 Potsdam, Germany — [2]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter EX4 4QL, UK — [3]Asia Pacific Center for Theoretical Physics, Pohang 37673, Republic of Korea

Pb on Si(111)-(7x7) has been subject of numerous studies due to its strong quantum size effect, which explains the height selection and the characteristic shape of coarsened islands [1]. Previous experiments have shown the fast nucleation and "explosive" growth of the Pb islands, which happens on a timescales much faster than explained by classical nucleation theory [2,3]. In this talk we focus on numerically modelling the mass transport onto a growing island, as a first step to find an explanation for the "explosive" island growth. Our simulations are motivated by a recent experiment, which locally triggers stable Pb islands to grow in height. We show that certain surface processes in the Pb/Si(111)-(7x7) are well-described and explained by classical diffusion models.

[1] Z. Kuntová et. al. Phys. Rev. B, **78** (2008)
[2] H. Hattab et. al. Surf. Sci. **646** (2016)
[3] M. Hershberger et. al. Phys. Rev. Lett., **113** (2014)

O 9.7 Mon 12:00 MA 144

An in-situ microGISAXS growth study of metallic thin films on self organized nanopatterned templates — •Sarathlal Koyiloth Vayalil[1,2], Praveen Kumar Dubey[2], Benedikt Sochor[1], Matthias Schwartzkopf[1], Stephan V. Roth[1], and Ajay Gupta[2] — [1]Deutsches Elektronen Synchrotron DESY, Notkestr. 85, 22607, Germany — [2]UPES, Bidholi Campus, Dehradun, 248007, Uttarakhand, India

In this work, a detailed insitu μGISAXS investigation of the growth of metallic thin films on self-organized nanopatterned templates prepared by low energy ion beam erosion has been done. GISAXS experiments were performed at the P03/MiNaXS beamline of the PETRA III storage ring at DESY (Hamburg, Germany).Two different kind of nanopatterned templates, (i) GaSb nanocones and (ii) nanorippled Si prepared by low energy ion beam erosion under two different experimental geometry have been used as templates to grow thin films of Py and Ag separately. Different growth regimes have been analyzed with increasing thickness. Obtained structural information have been correlated with observed variation in the functional properties of the thin films with increasing thickness values.