O 47: New methods: Theory

Time: Tuesday 14:30–15:30 Location: HSZ/0201

O 47.1 Tue 14:30 HSZ/0201

Energy-resolved tip-orbital fingerprint in scanning tunneling spectroscopy based on the revised Chen's derivative rule — Ivan Abilio[1,2] and •Krisztián Palotás[1] — [1]HUN-REN Wigner Research Center for Physics, Budapest, Hungary — [2]Budapest University of Technology and Economics, Budapest, Hungary

The revised Chen's derivative rule for electron tunneling [1] is implemented to enable computationally efficient first-principles-based calculations of the differential conductance dI/dV for scanning tunneling spectroscopy simulations [2]. By taking pristine and boron- or nitrogen-doped graphene sheets as sample surfaces, the reliability of our implementation is demonstrated by comparing its results to those obtained by the Tersoff-Hamann and Bardeen's electron tunneling models. It is highlighted that the energy-resolved direct and interference contributions to dI/dV arising from the tip's electron orbitals result in a fingerprint of the particular combined surface-tip system. The significant difference between the electron acceptor boron and donor nitrogen dopants in graphene is reflected in their dI/dV fingerprints. The presented theoretical method allows for an unprecedented physical understanding of the electron tunneling process in terms of tip-orbital-resolved energy-dependent dI/dV maps that is anticipated to be extremely useful for investigating the local electronic properties of novel material surfaces in the future. References: [1] Phys. Rev. B 91, 165406 (2015). [2] Phys. Rev. B 111, 245425 (2025).

O 47.2 Tue 14:45 HSZ/0201

Innovative Approaches to Semiconductor Surface Oxidation Studies Using Active Learning and MLIP — •Ondrej Krejci[1,2], Shola Adyemi[2], Konstantinos Konstantinou[2], and Milica Todorović[2] — [1]Department of Chemistry and Materials Science, Aalto University, Espoo, Finland — [2]Department of Mechanical and Materials Engineering, University of Turku, Turku, Finland

Oxygen passivation of InAs surfaces critically affects material performance in electronic devices, but the nature of the oxide surface reconstruction is not well characterized. To address this, we employ a machine learning (ML) driven workflow. Starting from the $\zeta(4\times2)$ reconstruction of pristine InAs(100) [1], we use Bayesian Optimization [2] to identify oxygen binding sites. This allows us to populate the surface with increasing number of oxygen atoms. The oxide models serve as input for a ML interatomic potential based on the MACE model [3], trained via the active learning method PALIRS [4]. The potential is used for molecular dynamics simulations to identify promising candidates for the oxidized InAs(100) surface reconstruction. Our workflow enables an efficient exploration of configurational space surpassing traditional computational approaches.

[1] Appl. Phys. A 75, 89 (2002)
[2] Npj. Comput. Mat. 5, 35 (2019)
[3] NeurIPS 35, 11423 (2022)
[4] Npj Comput. Mat. 11, 324 (2025)

O 47.3 Tue 15:00 HSZ/0201

Complete basis limit with hybrid functionals using LAPW — •Janis Uzulis and Andris Gulans — University of Latvia, Riga, Latvia

We present a systematic framework for achieving the complete basis limit (CBL) for molecules and solids in hybrid functional calculations with density functional theory using the linearized augmented plane wave (LAPW) method. Standard LAPW calculations with nonlocal exchange employ radial basis functions and core orbitals obtained from a (semi)local functional, leading to inconsistencies that prevent the calculations from converging to CBL. We address this issue and achieve the same level of precision that previously was attainable only with local functionals. By applying this method, we obtain the Hartree-Fock total energy for crystals with a few μHa precision. Aside from high-quality reference data (reaction energies, cohesive energies and equation of state) for computational-chemistry and band-structure codes, our work provides an insight into the range of applicability of the standard approach to hybrids in LAPW.

O 47.4 Tue 15:15 HSZ/0201

AI-Driven Optimization Techniques for Density Functional Theory Calculations — Álvaro Fraile-Carmena[1], Damián Sánchez-Maqueda[1], Cristian Ramírez-Atencia[1], and •María Camarasa-Gómez[2] — [1]Universidad Politécnica de Madrid, C/ Alan Turing, s/n, Madrid 28031, Spain — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Paseo de Manuel Lardizábal 5, Donostia-San Sebastián 20018, Spain

Accurately determining optoelectronic properties of molecules and solids is an ongoing challenge in first-principles methods. This objective has gained even more relevance, as research on quantum materials evolves rapidly. So far, density functional theory (DFT) has remained the primary computational tool for this task. However, reaching with DFT accuracy levels comparable to many-body perturbation theory still requires significant computational effort [1]. Here we introduce an approach that integrates AI-driven optimization techniques into DFT workflows [2]. Embedding these optimization methods directly in ab initio software enhances both accuracy and efficiency. We present results obtained with surrogate models and state-of-the-art open source optimization libraries [3], showing their potential to accelerate and improve electronic structure simulations. [1] M. Camarasa-Gómez, S. E. Gant, et al., npj Comput. Mater. 10, 288 (2024) [2] Á. Fraile-Carmona, D. Sánchez-Maqueda, C. Ramírez-Atencia, and M. Camarasa-Gómez (2025) [in preparation] [3] J. Blank, and K. Deb, IEEE Access 8, 89497 (2020)