MP 5: Theoretical Aspects of Condensed Matter I

Time: Monday 16:00–17:20 Location: HL 102

MP 5.1 Mon 16:00 HL 102

First-principles study of armchair SiS nanoribbons with F and Cl functionalization — •Rachana Yogi[1], Alok Shukla[1], and Neeraj K. Jaiswal[2] — [1]Department of Physics,Indian Institute of Technology Bombay, Powai, Mumbai 400076 India — [2]2D Materials Research Laboratory, Discipline of Physics, Indian Institute of Information Technology Design & Manufacturing, Jabalpur, 482005, India.

Fluorine (F) and Chlorine (Cl) are amongst the toxic gases which are highly reactive and hazardous to the environment. Therefore, to comprehend the quantum of lethality they pose, it is crucial to identify and quantify their concentration in substances. Accordingly, in the present research, the first-principles calculations based on density functional theory have been employed to reveal the structural stability, electronic and transport properties of armchair SiS nanoribbons (ASiSNR), functionalized with Cl, F and H. Our observations based on binding energy analysis suggest that all the considered structures are thermodynamically stable. It is also observed that the semiconducting behavior persists on passivation of Cl and F. However, the stability of the structure has enhanced compared to their bare and pristinecounterparts. our investigation on the transport properties of considered structures using the two-probe model revealed that the obtained current-voltage (I-V) characteristics have of current as a function of bias voltage. From these results, it is certain that the upcoming epochs of nano-electronic devices may use ASiSNR as a potential material for nano-electronics and chemical sensors.

MP 5.2 Mon 16:20 HL 102

Unidirectional Wave Propagation in a Topological Plasmonic Ring Resonator via a Symmetry-Broken Excitation Scheme — •Fatemeh Davoodi and Nahid Talebi — Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany

Topological plasmonics, at the intersection of topology and plasmonics, offers an innovative approach to light manipulation, leveraging the Su-Schrieffer-Heeger model to create resilient ring-shaped plasmonic chains with topologically protected edge modes. This study thoroughly investigates the design, characterization, and manipulation of these topological plasmonic chains comprised of nano-discs. Emphasis is placed on understanding the unique properties of resonators, particularly their potential to support topologically protected edge modes within rotationally symmetric optical modes in a ring geometry. Utilizing a symmetry-breaking excitation technique with electron beams, topological edge modes are observed in rotationally symmetric chains. We analyze the influence of parameters like dimerization and loop numbers on the presence of the Edge modes. Additionally, the electron impact is suggested as a parameter to control the direction of propagation and selectively excite specific bulk or edge modes. These findings hold important implications for the advancement of nanoscale plasmonic systems with tailored functionalities, and unidirectional propagation of light in topological ring resonators coupled to point-like emitters such as quantum dots and defect centers.

MP 5.3 Mon 16:40 HL 102

Semiclassical quantization of quantum plasmons in spatially inhomogeneous media — •Koen Reijnders, Timur Tudorovskiy, and Mikhail Katsnelson — Radboud University, Institute for Molecules and Materials, Nijmegen, The Netherlands

We present a novel semi-analytical method to describe plasmons, collective excitations of the conduction electrons in solids, in spatially inhomogeneous media. Since these systems do not exhibit translational invariance, the Fourier transform cannot be used to construct a solution. However, when we demand that the characteristic scale of the inhomogeneities is much larger than the plasmon wavelength, we can instead employ techniques taken from the semiclassical approximation. In this way, we construct an asymptotic solution that is independent of the precise shape of the inhomogeneity [1]. Technically, we study a system of equations of motion that is equivalent to the random phase approximation, and which can also be viewed as a quantum generalization of the Vlasov–Poisson system. We solve this system self-consistently using the correspondence between quantum mechanical operators and classical observables on phase space. In this way, we obtain a classical Hamiltonian that describes the dynamics of quantum plasmons, given by the Lindhard function with spatially varying parameters. We then find the energy levels using Bohr–Sommerfeld quantization. Our results provide a theoretical basis to describe plasmonic waveguides and other setups in quantum plasmonics.

[1] K. J. A. Reijnders, T. Tudorovskiy, M. I. Katsnelson, Ann. Phys. (NY) 446, 169116 (2022)

MP 5.4 Mon 17:00 HL 102

Autonomous atomic Hamiltonian construction and active sampling of X-ray absorption spectroscopy by adversarial bayesian optimization — •Yixuan Zhang[1], Ruiwen Xie[1], Teng Long[2], Damian Günzing[3], Heiko Wende[3], Katharina J.ollefs[3], and Hongbin Zhang[1] — [1]Institute of Materials Science, Technical University of Darmstadt, 64287, Darmstadt, Germany — [2]School of Materials Science and Engineering, Shandong University, 250061, Jinan, China — [3]Faculty of Physics, University of Duisburg-Essen, 47057, Duisburg, Germany

X-ray absorption spectroscopy (XAS) is a well-established method for in-depth characterization of electronic structure. In practice hundreds of energy-points should be sampled during the measurements, and most of them are redundant. Additionally, it is also tedious to estimate reasonable parameters in the atomic Hamiltonians for mechanistic understanding. We implement an Adversarial Bayesian Optimization (ABO) algorithm comprising two coupled BOs to automatically fit the many-body model Hamiltonians and to sample effectively based on active learning (AL). Taking NiO as an example, we find that less than 30 sampling points are sufficient to recover the complete XAS with the corresponding crystal field and charge transfer models, which can be selected based on intuitive hypothesis learning. Further applications on the experimental XAS spectra reveal that less than 80 sampling points give reasonable XAS and reliable atomic model parameters. Our ABO algorithm has a great potential for future applications on automated physics-driven XAS analysis and AL sampling.