O 53: Poster Electronic Structure Theory

Time: Tuesday 18:00–20:00 Location: P2

O 53.1 Tue 18:00 P2

Enhancing Efficiency of Bethe-Salpeter equation calculations including spin-orbit coupling — •Seokhyun Hong, Cecilia Vona, Sven Lubeck, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin

Calculating optical excitations in materials with significant spin-orbit coupling (SOC) effects is challenging due to the computational costs. We propose a new method to compute optical spectra including excitonic effects within an all-electron framework. This method extends recently introduced second variation with local orbital (SVLO) method[1] towards the Bethe-Salpeter equation (BSE) framework. The SVLO method is based on the conventional second variation (SV) approach for density-funtional theory calculations. In SV, SOC is treated as a perturbation through a two-step procedure. By solving the scalar relativistic (SR) Hamiltonian, we first obtain eigenvalues and states without SOC. A sub-set of these SR Kohn-Sham states is used as basis functions for evaluating the SOC terms. For many materials, this approach can require all available states for convergence and thus may not capture SOC effects accurately without resorting to huge matrix sizes. In the SVLO method, local orbitals (LOs) are included in the SV step as additional basis functions. It could be shown that this enhances the computational efficiency tremendously[1]. Through this work, we have implemented an analogous scheme in the BSE framework. We demonstrate, how we overcome current limitations and achieve highly precise results for materials with strong SOC, such as lead iodide, perovskites, MoS2,etc.

O 53.2 Tue 18:00 P2

First-Principles Calculations of X-ray Absorption Spectra: Supercell Core-Hole Method versus Bethe-Salpeter Equation — •Ziyu Wang[1], Lu Qiao[1], Ronaldo Rodrigues Pelá[2], and Claudia Draxl[1] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Zum Großen Windkanal 2, 12489 Berlin, Germany — [2]Supercomputing Department, Zuse Institute Berlin (ZIB), Berlin, Takustraße 7, 14195 Berlin, Germany

Accurate simulations of X-ray absorption spectra (XAS) are essential for understanding core-level excitations and electronic structure. In this study, we compare two approaches for calculating XAS: the supercell core-hole (SCH) method based on density-functional theory and the Bethe-Salpeter equation (BSE) of many-body perturbation theory. In the SCH method, core excitations are simulated by removing a core electron from the system, thus treating electron-hole interaction on the DFT level. In contrast, excitonic effects are considered explicitly in the two-body Hamiltonian underlying the BSE. We apply the SCH method with various exchange-correlation (xc) functionals of DFT to calculate XAS in diverse materials (metals, semiconductors, and insulators) and absorption edges. By comparing them with XAS obtained from BSE, we evaluate in which cases the SCH method is appropriate to be applied.