O 79: Poster Session - Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interaction

Time: Wednesday 18:15–20:00 Location: P2/EG

O 79.1 Wed 18:15 P2/EG

Photoexcited oxirane modelled by ab initio nonadiabatic molecular dynamics — •Marvin Krenz, Wolf Gero Schmidt, and Uwe Gerstmann — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn,Germany

Oxirane, C2H4O, is a prototypical model system to explore photoreactions [1] and theirtheoretical modelling [2]. In this study we explore the prowess of constrained density-functional theory (cDFT) for optically excited states [3] in conjunction with Tully's fewest switches surface hopping [4] in describing the dynamics of photoexcited oxirane. Using nonadiabatic molecular dynamics in the Libra-X implementation [5], we study the influence of the initial atomic temperature on the photoreactions of oxirane.

Different atomic temperatures are modelled by initial velocities as well as by using the Nosé-Hoover thermostat. The results are compared to experimental [1] and earlier theoretical findings [2]. It is found that the cDFT approach in conjunction with an a temperature description based on the initial atomic velocities well explains the measured data on the reaction path distribution, while the usage of the thermostat tends to slow down the reactions.

[1] M. I. Masahiro Kawasaki et. al., Chemical Physics (1973).

[2]U. R. C. F. Enrico Tapavicza et. al., Journal of Chemical Physics 129 (2008).

[3] T Frigge et al., Nature 544, 207 (2017).

[4] JC Tully, J. Chem. Phys 93, 1061 (1990).

[5] E Pradhan et al., J. Phys.: Condens. Matter 30, 484002 (2018).

O 79.2 Wed 18:15 P2/EG

Electronic and optical properties of $CoFe_2O_4$ and Co_3O_4 including many body effects — •Shohreh Rafiezadeh, Hamidreza Hajiyani, and Rossitza Pentcheva — Department of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg

Cobalt oxides such as $CoFe_2O_4$ play an important role as anode material for photocatalytic water splitting, necessitating detailed understanding of their optical properties. Here, we investigate the electronic and optical properties of $CoFe_2O_4$ and Co_3O_4 based on density functional theory (DFT) calculations. Previous experimental studies of $CoFe_2O_4$ have reported a wide range of values for both indirect and direct band gap between 0.9-1.5 eV and 2.0-2.76 eV, respectively. While DFT+U indicates a direct one (1.38 eV), an indirect band gap of 1.81 eV emerges when many body effects are included. Comparison of the real and imaginary part of the dielectric function within the independent-particle picture, G_0W_0 and by solving the Bethe-Salpeter equation (BSE) indicates the relevance of excitonic effects. Support by the German Science Foundation (DFG), CRC/TRR 247, project B04 and a computational grant at MagnitUDE are gratefully acknowledged.

O 79.3 Wed 18:15 P2/EG

Electron-phonon interaction in hybrid inorganic/organic systems: implementation within the LAPW formalism — •Ignacio Gonzalez Oliva, Fabio Caruso, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Electron-phonon interactions (EPI) are ubiquitous in condensed matter and manifest themselves in a wide range of physical phenomena, such as the temperature dependence of the electrical resistivity and the emergence of conventional superconductivity. While in the last decade computational tools to study EPI in crystalline solids from first principles have become accessible, their application to hybrid inorganic/organic systems (HIOS) and interfaces is still hindered by the high computational cost of EPI calculations. We are developing an effective first-principles approach to extend EPI calculations to HIOS. Considering the vibrational properties of the constituents, we include their effects in the electronic properties of the hybrid system. This approach is being implemented in the `exciting` code, a full-potential all-electron code based on the linearized augmented plane-wave plus local orbitals (LAPW + lo) method. We will present details on the implementation and first applications.

O 79.4 Wed 18:15 P2/EG

An efficient representation of the Kohn-Sham potential and its use in density functional calculations — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In the standard numerical treatment, the main effort is directed at an efficient description of the density, usually by applying a judicious expansion in basis functions or a sophisticated choice of numerical grid points. The potential $V(\underline{r})$ is then represented by its matrix elements determined by the basis functions or grid points. In view of the computational cost, this number is reduced as much as possible, often by replacing the real potential with a pseudopotential.

In my presentation, instead, the emphasis is put on an efficient description of the potential in terms of spherical harmonics used to expand the potential at the nuclear sites. The potential is understood as an integral operator $V(\underline{r})\delta(\underline{r}-\underline{r}')$ approximated by $\delta(r-r')\sum_{lml'm'} Y_{lm}(\underline{r})Y_{l'm'}(\underline{r}')V_{lml'm'}(r)$ with a finite number of spherical harmonics. For such potentials the density can be evaluated practically exactly by a mathematically rigorous expression [1]. The calculated densities converge fast with increasing number of harmonics and excellent total energies are obtained at low computational cost.

[1] R. Zeller, J. Phys.: Condens. Matter 27, 306301 (2015).

O 79.5 Wed 18:15 P2/EG

Adaptive meshes for Brillouin zone integrations — •Patrick Dieu[1], Maria Troppenz[2], and Claudia Draxl[3] — [1]Humboldt Universität zu Berlin, Germany — [2]Humboldt Universität zu Berlin, Germany — [3]Humboldt Universität zu Berlin, Germany

Adaptive schemes for selecting k-points in the Brillouin zone allow for accurate and efficient calculations of integrals in electronic-structure theory. Such techniques generate dense samplings in regions with high relevance for the integrand while maintaining a coarse grid in other regions. We implement a scheme for k-mesh refinement in the density-functional-theory package exciting [1] for the main purpose of calculating transport coefficients with high efficiency. The transport coefficients are obtained by solving the linearized Boltzmann equation [2]. Our method devides the Brillouin zone in cuboidal blocks with the k-points as vertices. We investigate the performance of this approach with respect to several parameters, e.g. the initial k-grid and different termination criteria of the algorithm. Our adaptive scheme can also be used for a precise determination of the Fermi surface. Overall, we demonstrate that this adaptive scheme saves a significant amount of computational time in comparison to methods using equispaced k-grids.

[1] A. Gulans, et al., J. Phys.: Condens. Matter 26, 363202 (2014).

[2] B. R. Nag; Electron Transport in Compound Semiconductors, Springer, New York, pp. 171-229 (1980).