

## HL 47: Theory of electronic structure

Time: Thursday 16:15–17:30

Location: EW 202

HL 47.1 Thu 16:15 EW 202

**Calculation of the bulk photovoltaic effect using maximally localized Wannier functions** — ●JULEN IBAÑEZ-AZPIROZ<sup>1</sup> and IVO SOUZA<sup>1,2</sup> — <sup>1</sup>Centro de Física de Materiales, Universidad del País Vasco, 20018 San Sebastián, Spain — <sup>2</sup>Ikerbasque Foundation, 48013 Bilbao, Spain

The bulk photovoltaic effect (BPVE), also known as the shift-current effect, is a nonlinear optical response that yields a net photocurrent in noncentrosymmetric crystals. Although the theory of the BPVE is well established, its practical implementation is challenging because it involves a subtle Berry-phase-like quantity [1]. Here we calculate the BPVE using a Wannier-interpolation scheme, which provides two main advantages over previous numerical schemes. First, it avoids summing over a complete set of virtual states, and hence it is free from truncation errors. Second, it allows for an efficient interpolation of the Brillouin-zone integrand onto a fine  $\mathbf{k}$ -point mesh, providing high accuracy and convergence. We test the Wannier interpolation of the BPVE in well studied systems including GaAs [1], BaTiO<sub>3</sub> [2] and several single-layer monochalcogenides [3]. Finally, we briefly discuss how our formalism relates to the tight-binding-based approach to the BPVE [4].

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[1] J. E. Sipe and A. I. Shkrebtii, PRB **61**, 5337 (2000) [2] S. M. Young and A. M. Rappe, PRL **109**, 116601 (2012) [3] T. Rangel *et al.*, PRL **119**, 067402 (2017) [4] A. M. Cook *et al.*, Nat. Comm. **8**, 14176 (2017)

HL 47.2 Thu 16:30 EW 202

**Dielectric response function in colloidal quantum dots: combining microscopic and macroscopic screening** — ●ANASTASIA KARPULEVICH<sup>1,2</sup>, HANH BUI<sup>1,2</sup>, ZHI WANG<sup>1,2</sup>, and GABRIEL BESTER<sup>1,2</sup> — <sup>1</sup>Institute of Physical Chemistry, Hamburg University, Grindelallee 117, D-20146 — <sup>2</sup>The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, D-22761

Dielectric environment profoundly affects the optical properties of colloidal quantum dots (QDs), and modelling of the screening effects remains a challenging task. The recently developed Atomic Effective Pseudopotential (AEP) method provides single-particle energies and wave functions with close to ab-initio quality for colloidal QDs with atomistic passivation [1]. Configuration Interaction (CI) approach was implemented on top of ground-state wave functions to investigate excitonic properties of QDs [2]. We have developed the norm-dependent screening using masking function [3] applied to the individual wave functions. The method offers the opportunity to treat electron-electron interactions fully in reciprocal space, which considerably speeds up calculations, and considers both macroscopic (long-range) and microscopic (short-range) screening effects. The high-level transferability on different semiconductor materials and the influence of the non-polar solvents on the exciton binding energy were demonstrated. The obtained results were compared to the low-temperature experiments as well as to other CI-based models. [1] Karpulevich A. *et al.* (2016) Phys.Rev.B, 94 [2] Franceschetti A. and Zunger, A. (2000) Phys.Rev.B, 62 [3] Cartoixa X. and Wang L.W. (2005) Phys.Rev.Lett., 94

HL 47.3 Thu 16:45 EW 202

**Empirical Band Gap Correction for DFT based Calculations** — ●JENS HÜHNERT<sup>1,2</sup>, ANASTASIA KARPULEVICH<sup>1,2</sup>, and GABRIEL

BESTER<sup>1,2</sup> — <sup>1</sup>Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, D-20146 Hamburg, Germany — <sup>2</sup>The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, D-22761 Hamburg, Germany

An empirical correction scheme is used on DFT-based effective pseudopotential calculations to reproduce the experimental bulk band structure of II-VI (CdTe, ZnTe) and III-V (InAs, GaAs, GaP) semiconductors. The local potential as well as the non-local potentials can be corrected with a maximum of 4 parameters. The main focus of the correction is the band gap and the effective electron mass. It will be shown on the example of InAs that the bulk correction is transferrable to quantum dots to reach a good agreement with experimental results.

HL 47.4 Thu 17:00 EW 202

**Optical properties of NV centres using combined DFT/configuration interaction** — ●WALTER PFÄFFLE<sup>1,3</sup>, DENIS ANTONOV<sup>2</sup>, JÖRG WACHTRUP<sup>2</sup>, and GABRIEL BESTER<sup>1,3</sup> — <sup>1</sup>Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, D-20146 Hamburg, Germany — <sup>2</sup>Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart, Germany — <sup>3</sup>The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, D-22761 Hamburg, Germany

Configuration Interaction (CI) is a well established and widely used approach for solving the electronic Schrödinger equation including many-body correlations. Using wave functions obtained from density functional theory leads to an intricate double counting (DC) problem. We investigate the DC issue and derive an appropriate restricted CI Hamiltonian. The developed calculation scheme is applied to predict the many-body energy levels of the neutral, negatively and positively charged nitrogen vacancy centres in diamond.

HL 47.5 Thu 17:15 EW 202

**Excitonic optical spectra from a GW-free Bethe-Salpeter Equation** — ●JOSHUA ELLIOTT<sup>1,2</sup>, NICOLA COLONNA<sup>3</sup>, MARGHERITA MARSILI<sup>1</sup>, NICOLA MARZARI<sup>3</sup>, and PAOLO UMARI<sup>1</sup> — <sup>1</sup>Dipartimento di Fisica e Astronomia, Università degli studi di Padova, Padova Italy — <sup>2</sup>CNR-IOM DEMOCRITOS, Consiglio Nazionale delle Ricerche-Istituto Officina dei Materiali, c/o SISSA, Trieste, Italy — <sup>3</sup>Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

We present our recent implementation that combines Koopman's compliant (KC) Density Functionals with the Bethe-Salpeter Equation (BSE). Our method may be used to compute the optical properties of materials including excitonic effects, avoiding the costly GW-approximation. In this proof-of-concept work, quasiparticle eigenvalues are obtained perturbatively from the KC functional. Thus we use as input for the BSE: Kohn-Sham wavefunctions with quasiparticle-corrected energies, roughly equivalent to one-shot  $G_0W_0$ +BSE calculations. In addition, within the BSE calculation, we introduce a new method for obtaining the exact screened Coulomb interaction directly. This new approach has multiple advantages: it removes the need to compute the screened Coulomb interaction matrix,  $W(\mathbf{r}, \mathbf{r}')$ , further driving down the overall computation time and reducing the number of user-defined parameters. We evaluate the performance of our current implementation in the context of Thiel's set, a collection of 28 organic molecules.