

Optical and core spectroscopy from many-body perturbation theory

Caterina Cocchi

Physics Department, Humboldt-Universität zu Berlin, Germany

e-mail: caterina.cocchi@physik.hu-berlin.de

First-principles methods based on density-functional theory and many-body perturbation theory are the state-of-the-art approaches to study light-matter interaction at the nanoscale. All-electron implementations, like the one provided in the **exciting** code [1], offer the additional advantage to treat on the same footing optical and core excitations [2]. After introducing the underlying methodology, I will discuss the role of correlation effects that are essential for a quantitative description of light-absorption phenomena and yet act rather differently in transitions to unoccupied states from valence and core electrons. To illustrate this point, I will present selected examples from my recent research, addressing optical and core spectroscopy in inorganic [2,3], organic [4-6], and hybrid materials [7,8].

References:

- [1] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, and C. Draxl, *J. Phys.: Condens. Matter* **26**, 363202 (2014).
- [2] C. Vorwerk, C. Cocchi, and C. Draxl, *Phys. Rev. B* **95**, 155121 (2017).
- [3] C. Cocchi, S. Mistry, M. Schmeisser, J. Kühn, T. Kamps *J. Phys.: Condens. Matter*, *in press* (2018), arXiv:1809.00135.
- [3] C. Cocchi, and C. Draxl, *Phys. Rev. B* **92**, 205105 (2015).
- [4] C. Cocchi, T. Moldt, C. Gahl, M. Weinelt, and C. Draxl, *J. Chem. Phys.* **145**, 234701 (2016).
- [5] C. Cocchi, and C. Draxl, *J. Phys.: Condens. Matter* **29**, 394005 (2017).
- [6] C. Vorwerk, C. Hartmann, C. Cocchi, G. Sadoughi, S. N. Habisreutinger, R. Félix, R. G. Wilks, H. J. Snaith, M. Bär, and C. Draxl, *J. Phys. Chem. Lett.* **9**, 1852 (2018).
- [7] O. Turkina, D. Nabok, A. Gulans, C. Cocchi, and C. Draxl, *Adv. Theory Simul.*, 1800108 (2018), DOI: 10.1002/adts.201800108.