SFB1242

SFB 1242 Nichtgleichgewichtsdynamik kondensierter Materie in der Zeitdomäne

UNIVERSITÄT DUISBURG ESSEN

Open-Minded

27.11.2018 / 10 Uhr c.t., Raum MG 272
Campus Duisburg

Light-matter interaction from first principles in the linear regime and beyond

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Understanding how materials interact with electromagnetic radiation offers a unique perspective on their intrinsic physical properties. First-principles methods are particularly suited to this purpose, as they allow for a reliable description of the electronic structure without depending on empirical parameters. I will demonstrate the predictive power of (time-dependent) density-functional theory and many-body perturbation theory (including the GW method and the Bethe-Salpeter equation) in an overview on my recent research, embracing different kinds of systems and addressing various spectroscopic processes. First, I will focus on optical and x-ray absorption in molecular materials [1-6], where the interplay between intra- and inter-molecular interactions crucially determines the nature of the excitations. Next, I will turn to the nonlinear response of conjugated molecules and present a novel ab initio approach to calculate optical power limiting in good agreement with experiments [7]. Finally, I will demonstrate that the insight on the electronic structure offered by first-principles methods is essential for characterizing novel materials for electron sources and for modelling their photoemission properties [8].

References

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[3] C. Cocchi and C. Draxl, J. Phys.: Condens. Matter. **29**, 394005 (2017).
[4] C. Cocchi, T. Breuer, G. Witte, and C. Draxl, submitted (2018).
[5] A. M. Valencia and C. Cocchi, to be submitted.
[6] M. Guerrini, C. Cocchi, A. Calzolari, D. Varsano, and S. Corni, in preparation.
[7] C. Cocchi, D. Prezzi, A. Ruini, E. Molinari, and C. A. Rozzi, Phys. Rev. Lett. **112**, 198303 (2014).
[8] C. Cocchi, S. Mistry, M. Schmeißer, J. Kühn, and T, Kamps, submitted (2018); arXiv: 1809.00135.

Für diese Zeit steht eine Kinderbetreuung nach vorheriger Anmeldung zur Verfügung.

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