Contribution submission to the conference Berlin 2018

Coupling Maxwell's equations to the time-dependent Kohn-Sham equations: near-field effects and electromagnetic backreaction — •René Jestädt[a], Micael Oliveira[a], Angel Rubio[a,b,c], and Heiko Appel[a] — [a]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Germany — [b]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, USA — [c]Nano-bio Spectroscopy Group and ETSF, Universidad del País Vasco, 20018 San Sebastián, Spain

Induced currents in large molecular and condensed matter systems are non-negligible and can affect the conductivity and the optical properties of the system. In the present work, we have implemented the real-time propagation of Maxwell's equations in Riemann-Silberstein representation [1] to use standard unitary propagation techniques in the TDDFT code octopus [2]. The Maxwell and the Kohn-Sham system are coupled via a predictor-corrector method to obtain a self-consistent time-evolution of the total system [3]. Explicitely solving the microscopic Maxwell's equations also allows us to determine the optical properties of the system directly from the Maxwell fields. We show near-field effects of a full Maxwell-matter and matter-Maxwell coupling for plasmon excitations in metallic nanoparticles [3,4] and for ring-currents in organic molecules [3]. [1] I. Bialynicki-Birula, Progress in Optics **36**, 245-294 (1996)
[2] Alejandro Varas et al., J. Phys. Chem. Lett. 2015, **6**, 1891-1898
[3] R. Jestädt et al., (to be submitted) [4] X. Andrade et al., Physical

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Part:	**O**
Type:	**Vortrag;Talk**
Topic:	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials**
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