

## Real-time propagation of a Na<sub>297</sub> dimer as a coupled Maxwell-Schrödinger and time-dependent Kohn-Sham-Maxwell system

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External electromagnetic fields can induce non-negligible electric currents which influence the total Maxwell fields inside molecular systems. This backreaction affects the conductivity and the optical properties of molecular and nanoplasmonic systems. In the present work, we employ the Riemann-Silberstein vector of the electromagnetic field to cast Maxwell's equations into a spinor representation similar to the Dirac equation [1]. This representation allows us to use standard unitary propagation techniques [2], both for Maxwell's equations and the time-dependent Kohn-Sham equations. To illustrate our novel implementation of the coupled Maxwell-Kohn-Sham equations in the real-space code octopus [3], we show the effects of a large matter feedback to the Maxwell fields and vice versa a radiation feedback to electrons and nuclei for a Na<sub>297</sub> nanoparticle.

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[3] X. Andrade et al., J. Phys. Cond. Mat. **24**, 233202, (2012).