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Simulating Excitons in MoS2 with Time-Dependent Density Functional Theory CEDRIC FLAMANT, GRIGORY KOLESOV, EFTHIMIOS KAXIRAS, Harvard University — Monolayer molybdenum disulfide, owing to its graphene-like two-dimensional geometry whilst still having a finite bandgap, is a material of great interest in condensed matter physics and for potential application in electronic devices. In particular, MoS2 exhibits significant excitonic effects, a desirable quality for fundamental many-body research. Time-dependent density functional theory (TD-DFT) allows us to simulate dynamical effects as well as temperature-based effects in a natural way given the direct treatment of the time evolution of the system. We present a TD-DFT study of monolayer MoS2 exciton dynamics, examining various qualitative and quantitative predictions in pure samples and in the presence of defects. In particular, we generate an absorption spectrum through simulated pulse excitation for comparison to experiment and also analyze the response of the exciton in an external electric field.In this work we also discuss the electronic structure of the exciton in MoS2 with and without vacancies.

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