

Abstract Submitted  
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**Excitons in solids with non-empirical hybrid time-dependent density-functional theory**<sup>1</sup> CARSTEN ULLRICH, University of Missouri, ZENG-HUI YANG, Temple University, FRANCESCO SOTTILE, ETSF, Ecole Polytechnique, Palaiseau — The Bethe-Salpeter equation (BSE) accurately describes the optical properties of solids, but is computationally expensive. Time-dependent density-functional theory (TDDFT) is more efficient, but standard functionals do not produce excitons in extended systems. We present a new, non-empirical hybrid TDDFT approach whose computational cost is much less than BSE, while the accuracy for both bound excitons and the continuum spectra is comparable to that of the BSE. Good performance is observed for both small-gap semiconductors and large-gap insulators.

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