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Assessment of long-range-corrected exchange-correlation kernels for solids: Accurate exciton binding energies via an empirically scaled Bootstrap kernel

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In time-dependent density-functional theory, a family of exchange-correlation kernels, known as long-range-corrected (LRC) kernels, have shown promising, but conflicting [1–4] results for excitonic effects in solids. To address the issue, we perform a systematic assessment of existing static LRC kernels for a wide range of semiconducting and insulating solids, focusing on optical spectra and exciton binding energies. [5] We find that no LRC kernel is capable of simultaneously producing good optical spectra and accurate exciton binding energies for both semiconductors and insulators. We propose a simple and universal, empirically scaled Bootstrap kernel which yields accurate exciton binding energies for all materials under consideration. Finally, we discuss possible ways to overcome the fundamental and practical limitations of the LRC kernel.

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