Abstract Submitted
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Phonon dispersion of acene molecular crystals using van der Waals-corrected density functional theory[1] FLORIAN ALTVATER, University of California, Berkeley, TONATIUH RANGEL, Lawrence Berkeley National Laboratory, JEFFREY B. NEATON, University of California, Berkeley; Lawrence Berkeley National Laboratory — Acene molecular crystals are interesting testbeds for the study of phenomena relevant to organic optoelectronics, including charge separation and carrier transport. In such processes, scattering from lattice vibrations is an important dissipation mechanism. Despite their central role in dissipation processes, there are few calculations of phonon spectra in acene crystals. Here, we carry out van der Waals-corrected density functional theory calculations of the ground-state structure and phonon band structure of acene molecular crystals, comparing to neutron diffraction data where applicable. We use a finite-differences method, and compare the performance of several approaches – including standard generalized gradient approximations (GGA) such as PBE, PBE plus pair-wise vdW corrections, and vdW density functionals – to experiments for solid naphthalene and pentacene.

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