Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Phonon dispersion in acene molecular crystals using van der Waals density functionals FLORIAN BROWN-ALTVATER, University of California, Berkeley, TONATIUH RANGEL, Lawrence Berkeley National Laboratory, JEFFREY B. NEATON, University of California, Berkeley; Lawrence Berkeley National Laboratory — Much progress has been made of late in understanding the fundamental processes in optoelectronic materials. An ongoing challenge is the accurate inclusion of nuclear motion and to go beyond the Born-Oppenheimer approximation. Especially in materials like molecular crystals, where van der Waals (vdW) forces dominate the cohesive energy and the electronic structure is very sensitive to intermolecular geometry, phonons can be an important facilitator and dissipation mechanism. Thus there is a need to assess and understand the efficacy of existing approaches for phonon dispersions in vdW-bound solids. In this work we use a vdW density functional to calculate the phonon dispersion of members of the acene family. We establish the accuracy of the method using naphthalene, obtaining excellent agreement with experimental results, and in a further step, we explore the strength of the electron-phonon coupling across the Brillouin zone. Taken all together, our calculations illustrate the potential for quantitative prediction of vibrational properties of weakly-bound organic crystals over the entire Brillouin zone from first principles.

Florian Brown-Altvater
Univ of California - Berkeley

Date submitted: 05 Nov 2015 Electronic form version 1.4