Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

**Band gap renormalization and temperature dependence of acene crystals: the case of naphthalene** F. BROWN-ALTVATER, T. RANGEL, Univ of California - Berkeley, Lawrence Berkeley National Lab, G. ANTONIUS, Univ of California - Berkeley, M. GIANTOMASSI, Y. GILLET, Univ de Louvain, S. G. LOUIE, Univ of California - Berkeley, X. GONZE, Univ de Louvain, J. B. NEATON, Univ of California - Berkeley, Lawrence Berkeley National Lab — The band gap is one of the defining properties for semiconductors and insulators. It determines the energy of absorbed light in photovoltaic devices, the color of light emitting materials, or the redox potential for electrochemical reactions. Being able to accurately predict the band gap (its value and the position of the band edge states with respect to the vacuum level) is thus paramount for the design of new optoelectronic materials. Electronic structure theory has made big leaps towards this goal with ever improving functionals within the density functional formalism and many-body theories. The renormalization of the band structure due to electron-phonon interactions becomes equally important at finite as well as zero temperature. However, the computation of electron-phonon renormalization in molecular crystals is challenging, due to the small dispersion of the bands. Through improved algorithms and taking advantage of symmetries, we calculate the electron-phonon coupling in crystalline naphthalene from first principles using van der Waals density functionals, and determine the zero-point renormalization and temperature dependence of the electronic eigenstates within the Allen-Heine-Cardona theory.

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Date submitted: 28 Feb 2017 Electronic form version 1.4