

Abstract Submitted  
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**Van der Waals Dispersion Interactions and Excited States of Oligoacene Molecular Crystals**<sup>1</sup> TONATIUH RANGEL GORDILLO, SAHAR SHARIFZADEH, Molecular Foundry, LBNL, KRISTIAN BERLAND, Chalmers University of Technology, Sweden, FLORIAN ALTVATER, Molecular Foundry, LBNL; UC-Berkeley, KYUHO LEE, Molecular Foundry, LBNL, PER HYLDGAARD, Chalmers University of Technology, Sweden, LEEOR KRONIK, Weizmann Institute of Science, Israel, JEFFREY B. NEATON, Molecular Foundry, LBNL; UC-Berkeley — Molecular crystals are a prototypical class of van der Waals (vdWs)-bound organic materials with novel excited state properties relevant for photovoltaics applications. Predicting the structure and excited state properties of oligoacene crystals presents a challenge for standard density functional theory (DFT), as standard functionals do not have long-range dispersion, and DFT does not yield excited-state properties. In this work, we use a combination of vdW-corrected DFT – both pair-wise correction methods and correlation functionals – and many-body perturbation theory to study the geometry and excited states of oligoacene crystals. We find that vdWs methods can predict lattice constants up to 1% of the experimental measurements. Low lying excited states computed with MBPT compare well with experiments, and are found to be quite sensitive to geometry. Our study reveals the importance of vdWs dispersion interactions to the determination of excited states; moreover, our work suggests routes for predictive calculations, in which both structures and excited states are calculated entirely from first-principles.

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