Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Theoretical and experimental electronic structure of quinacridone SIVAN REFAELY-ABRAMSON, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth, Israel, DANIEL LUEFTNER, Institute of Physics, University of Graz, Graz, Austria, MICHAEL PACHLER, Institute of Physics, University of Graz, Graz, Austria; Institute of Solid State Physics, Graz University of Technology, Graz, Austria, ROLAND RESEL, Institute of Solid State Physics, Graz University of Technology, Graz, Austria, MICHAEL G. RAMSEY, Institute of Physics, University of Graz, Graz, Austria, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth, Israel, PETER PUSCHNIG, Institute of Physics, University of Graz, Graz, Austria
— Although density functional theory is often used to study the frontier energy levels of organic electronic materials, standard functionals tend to predict too small fundamental gaps, may lead to wrong orbital energy ordering, and do not capture polarization-induced gap renormalization. We examine a strategy for overcoming these issues by studying the gas phase and bulk electronic structure of the organic molecule quinacridone, a promising material for organic devices. We employ the recently developed optimally tuned screened range-separated hybrid (OT-SRSH) functional [PRB 88, 081204(R) (2013)], where the electronic screening is taken into account, and compare with angle-resolved photoemission spectroscopy on multilayers of quinacridone. Our method leads to the desired band gap renormalization and results in a valence band spectrum in excellent agreement with experimental data and with full-frequency G0W0 results based on a hybrid functional starting point. [PRB 90, 075204 (2014)]

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Date submitted: 13 Nov 2014 Electronic form version 1.4