Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Quantitative prediction of optical absorption in molecular solids using an optimally tuned screened range-separated hybrid functional ARUN K. MANNA, Weizmann Institute of Science, SIVAN REFAELY-ABRAMSON, University of California, ANTHONY REILLY, The Cambridge Crystallographic Data Centre, ALEXANDRE TKATCHENKO, University of Luxembourg, JEFFREY B. NEATON, University of California, LEEOR KRONIK, Weizmann Institute of Science — Quantitative prediction of optical absorption in the solid-state using density functional theory (DFT) is a long-standing challenge. In principle, this should be possible with time-dependent DFT (TDDFT). In practice, the results depend very strongly on the approximate exchange-correlation functional and standard approximations usually fail qualitatively in the solid state. We show that such prediction is possible, using the recently-developed time-dependent optimally-tuned screenedrange-separated hybrid (OT-SRSH). In this method the molecular electronic structure is determined by optimal tuning of the range-separation parameter in a range-separated hybrid functional. Screening and polarization in the solid-state are taken into account by adding long-range dielectric screening to the functional form. We provide a comprehensive benchmark for the accuracy of this approach, by considering the X23 benchmark set of molecular solids. The results are in good agreement with many-body perturbation theory in the GW-BSE approximation. We discuss strengths and weaknesses of the approach. We believe that it could be used for studies of molecular solids typically outside the reach of computationally more intensive methods.

Arun K. Manna
Weizmann Institute of Science

Date submitted: 13 Nov 2016 Electronic form version 1.4