Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Excitons in solids with time-dependent density-functional theory: the bootstrap kernel and beyond[1] YOUNG-MOO BYUN, Univ of Missouri - Columbia, ZENG-HUI YANG, Temple University, CARSTEN ULLRICH, Univ of Missouri - Columbia — Time-dependent density-functional theory (TDDFT) is an efficient method to describe the optical properties of solids. Lately, a series of bootstrap-type exchange-correlation (xc) kernels have been reported to produce accurate excitons in solids, but different bootstrap-type kernels exist in the literature, with mixed results. In this presentation, we reveal the origin of the confusion and show a new empirical TDDFT xc kernel to compute excitonic properties of semiconductors and insulators efficiently and accurately. Our method can be used for high-throughput screening calculations and large unit cell calculations.

[1]Work supported by NSF Grant DMR-1408904

Young-Moo Byun
Univ of Missouri - Columbia

Date submitted: 05 Nov 2015 Electronic form version 1.4