Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Efficient parameter-free calculation of absorption spectra for insulators, semiconductors and metals from time-dependent current DFT ARJAN BERGER, LCPQ - IRSAMC, Université de Toulouse III - Paul Sabatier, CNRS, Toulouse, France and European Theoretical Spectroscopy Facility — In this work we show that with a simple dynamical kernel we can obtain good absorption spectra from time-dependent current-density functional theory (TDCDFT) for insulators, semiconductors and metals. Our approach is fully parameter free since no artificial broadening parameter is used to match calculated and measured spectra. The cost of a calculation is equal to an RPA calculation. Moreover, our TDCDFT approach scales better with system size than standard TDDFT implementations.

Arjan Berger
LCPQ - IRSAMC, Université de Toulouse III - Paul Sabatier,
CNRS, Toulouse, France and European Theoretical Spectroscopy Facility

Date submitted: 13 Nov 2014 Electronic form version 1.4