Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Time-dependent potential-functional embedding theory CHEN HUANG, Department of Scientific Computing, Florida State University, USA, FLORIAN LIBISCH, Institute for Theoretical Physics, Vienna University of Technology, Austria, QING PENG, Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, USA, EMILY CARTER, Department of Mechanical and Aerospace Engineering, Princeton University, USA — We introduce a time-dependent potential-functional embedding theory (TD-PFET), in which atoms are grouped into subsystems. In TD-PFET, subsystems can be propagated by different suitable time-dependent quantum mechanical methods and their interactions can be treated in a seamless, first-principles manner. TD-PFET is formulated based on the time-dependent quantum mechanics variational principle. The action of the total quantum system is written as a functional of the time-dependent embedding potential, i.e., a potential-functional formulation. We derive the integral equation that such an embedding potential needs to satisfy. As proof-of-principle, we demonstrate TD-PFET for a Na4 cluster, in which each Na atom is treated as one subsystem and propagated by time-dependent Kohn-Sham density functional theory (TDDFT) using the adiabatic local density approximation (ALDA). Our results agree well with a direct TDDFT calculation on the whole Na4 cluster using ALDA. We envision that TD-PFET will ultimately be useful for studying ultrafast quantum dynamics in condensed matter, where key regions are solved by highly accurate time-dependent quantum mechanics methods, and unimportant regions are solved by faster, less accurate methods.

Chen Huang
Department of Scientific Computing, Florida State University

Date submitted: 13 Nov 2014 Electronic form version 1.4