Incorporating a new parallel quantum mechanical worker in the PUPIL system

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Abstract

PUPIL (Program for User Package Interfacing and Linking) is an open-source software package and set of protocols for systematic inter-operation of existing codes ("workers") for multi-threaded, multi-scale quantum-classical mechanical simulations (QM/MD). One part of the PUPIL design is use of minimally intrusive wrappers for each worker. Since the main bottleneck in this kind of simulation is clearly the quantum mechanical calculation, developing new interfaces with existing, highly parallelized QM applications opens the possibility of performing more realistic and complex multi-scale simulations. Thus motivated, we have incorporated the deMon2k suite as a new QM worker in PUPIL to provide an efficient parallel DFT code. Our demonstration study is the doped 3,4-ethylenedioxythiophen oligomer (PEDOT) in explicit acetonitrile. From a relatively short QM/MD run, we present electronic properties such as ionization potentials and energy gap are compared for non-doped and doped systems. The new wrapper for deMon2k, will be available from the PUPIL distribution site, http://pupil.sourceforge.net. [OB and JT was supported in part by MEC MAT2006-04029 and SBT by US NSF DMR0325553]