The PW-TELEMAN open-source library of GPU routines for molecular dynamics coupled to time-dependent density functional theory : performance and applications to clusters and molecules of biological interest

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We discuss the performance on various typical cases of a Time Dependent Density Functional Theory (TDDFT) library of codes with Self-Interaction Correction (SIC) nonadiabatically coupled to molecular dynamics (MD), intended for molecules and clusters. The library of codes, named PWTELEMAN, is open-sourced, scriptable under the common ASE (Atomic Simulation Environment) and optimized for modern Graphical Processing Units (GPU) architectures.

It is especially well suited to the study of irradiation effects, interactions of matter with intense femtosecond laser pulses or energetic ions. Such observables as the Photoemission spectroscopy (PES) can be easily computed. We discuss the implementation and compare the performance, scaling and precision of the PWTELEMAN code to various other TDDFT codes, linearized or not. The cases under study range from simple molecules and clusters such as the dihydrogen molecule or small sodium clusters up to molecules of biological interest such as fragment of proteins or clusters embedded in a matrix thanks to a QM/MM approach.