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Multi-domain decomposition method for real-time propagation of wave function[1] VLADIMIR GONCHAROV, KALMAN VARGA, Vanderbilt University — Extension of electronic structure methods to ever-large systems is an important problem in computational material and bio sciences. We have developed a time-dependent density functional approach that is capable to describe electron dynamics in large molecular complexes and realistic nanostructures. For wave function propagation, the most expensive numeric operation is the evaluation of product of Hamiltonian matrix and wave function. We use a multi-domain decomposition to increase numerical efficiency of this operation that results in efficient real time propagation of wave function in real space. We currently perform extensive testing of the new system and plan to use it in calculations of optical absorption spectra of supra-molecular assemblies. Results will be presented for C60-Fe-porphyrin complex.

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