Abstract Submitted
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Exact-Exchange Optimized Effective Potential and Memory Effect in Time-dependent Density Functional theory[1] SHENG-LUN LIAO, National Taiwan University, TAK-SAN HO, HERSCHEL RABITZ, Princeton University, SHIH-I CHU, University of Kansas — Nowadays, time-dependent density functional theory (TDDFT) is an efficient and accurate theoretical method to explore the ultrafast many-electron dynamic of atomic and molecular systems. However, most of TDDDT applications are limited to the adiabatic approximation, of which the important memory effect is neglected. To go beyond the adiabatic approximation, we derive a Sturm-Liouville-type time-local TDOEP equation for the construction of memory-dependent exchange-correlation (xc) potential associated with orbital-dependent functionals [1]. The non-adiabatic calculations for a one-dimensional two-electron Helium model are performed by using the time-local TDOEP equation with the exact exchange functional. The time-dependent dipole moment and probability density show that the TDOEP approach is more accurate than the Krieger-Li-Iafrate (KLI) approximation and the adiabatic local spin density approximation. In particular, the non-adiabatic and memory-dependent terms in the time-local TDOEP equation describe the time-dependent structure of xc potential properly. [1] S.-L. Liao, T.-S. Ho, H. Rabitz, and S.-I. Chu, Phys. Rev. Lett. 118, 243001 (2017).

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