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Transferability of Fragments in Partition Density Functional Theory YU ZHANG, ADAM WASSERMAN, Dept. of Chemistry, Purdue University — Partition Density Functional Theory (PDFT) is a method for calculating molecular properties from Kohn-Sham calculations on isolated fragments [P. Elliott, K. Burke, M.H. Cohen, and A. Wasserman, arXiv:0901.0942]. For a given choice of fragmentation, PDFT outputs the (in principle exact) molecular energy and density, as well as fragment densities that add up to the correct molecular density. Using a simple one-dimensional model system, we investigate the transferability of the resulting fragment densities by examining how their shape and dipole are preserved as the environment changes. Our results show that the PDFT fragment densities are in general more transferable than those arising from other popular density-partitioning schemes.

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