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Time-dependent Partition Density-functional Theory MARTIN MOSQUERA, ADAM WASSERMAN, Purdue University — We present an extension of time-dependent density functional theory that allows to partition the time-dependent external potential in terms of localized molecular fragment potentials. As a consequence, localized time-dependent densities arise for each molecular fragment. To enforce the condition that the sum of fragments must add up to the exact total density, a new quantity termed "time-dependent partition potential" is introduced. The Runge-Gross theorem is employed to show that there is a quasi one-to-one correspondence between the partition potential and the electronic density. The corresponding quantum-mechanical actions are derived by using the van Leeuwen's action and are used to derive a decomposition of the partition potential which allows for practical approximations. Linear response formulas are deduced to obtain the transition energies, and an approximation is suggested to obtain localized excitations in large molecular systems. Finally, numerical illustration of our theory is shown for one-dimensional fermions under the influence of a laser field.

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