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Recovering the Integer Discontinuity of Density Functional Approximations MARTIN MOSQUERA, Department of Chemistry, Purdue University, ADAM WASSERMAN, Purdue University — The derivative discontinuity (DD) of the exchange-correlation (XC) energy of density functional theory (DFT) is a consequence of the piece-wise linear dependency of the energy functional on the number of electrons of atoms or fragments that have been separated adiabatically from a molecule. Most approximations to the XC energy functional as the local-density approximation, the generalized-gradient approximation, exact exchange, among others, miss the DD or the piece-wise linear behavior, leading to inconsistencies in the analysis of molecular dissociation. We derive formal properties of the *exact* XC energy functional that lead to a framework to correct *any* density-functional approximation to display the required piece-wise linear dependency on the number of electrons and the DD. We will also illustrate how new approximation to the XC energy functionals can be developed for applications in DFT and fragment-based extensions.

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