

Abstract Submitted  
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**Ensemble treatment of fragments within a molecule leads to improved description of dissociation**<sup>1</sup> JONATHAN NAFZIGER, ADAM WASSERMAN, Purdue University — Approximate XC-functionals in Kohn-Sham (KS) density-functional theory (DFT) often fail when describing dissociation processes. This is due to improper treatment of fractional charges and spins within the dissociating systems. We demonstrate how the alternative framework of partition density-functional theory (PDFT) can correctly describe bond dissociation through its ensemble treatment of fragments within molecules. This method is illustrated through calculations on the dissociation of diatomic molecules.

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Jonathan Nafziger  
Purdue Univ

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