Abstract Submitted
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Van der Waals Interactions Between Subsystems with Overlapping Electron Density MICHELE PAVANELLO, Rutgers University — We claim that a subsystem formulation of Density-Functional Theory (DFT) can simplify both the theoretical framework and the computational effort for calculating the electronic structure of condensed phase systems. In addition, the naturally subsystem-like form of molecular aggregates makes subsystem DFT a better descriptor of the underlying physics than regular DFT of the supersystem. As an example, we present a novel van der Waals theory based on subsystem DFT which can treat seamlessly non-overlapping as well as overlapping subsystem electron densities. The theory is amenable to sensible approximations, such as RPA, and offers natural algorithms to fold in post-RPA corrections. Application of the theory to the computation of binding energies of dimers in the S22 set, and computation of selected potential energy surfaces is presented. [1] “FDE-vdW: A van der Waals Inclusive Subsystem Density-Functional Theory”, J. Chem. Phys., 141, 044127 (2014) [2] “Exact Kinetic Energy Enables Accurate Evaluation of Weak Interactions by the FDE-vdW Method”, J. Chem. Phys., 143, 084120 (2015) [3] “Subsystem Density-Functional Theory as an Effective Tool for Modeling Ground and Excited States, their Dynamics, and Many-Body Interactions”, J. Phys.: Condens. Matter, 27, 183202 (2015)

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