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Van der Waals Interactions Between Subsystems with Overlapping Electron Density[1] MICHELE PAVANELLO, Rutgers Univ - Newark — The subsystem formulation of DFT known as Frozen Density Embedding (FDE) provides a divide-and-conquer approach to Kohn–Sham DFT for weakly bound systems. We claim that a subsystem formulation of 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, as well as computation of selected potential energy surfaces is presented.

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