

Abstract Submitted
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Ab-Initio Modeling of Embedded Subsystems that Exchange Energy and Charge with the Environment MICHELE PAVANELLO, Rutgers University-Newark — We claim that a subsystem formulation of Density-Functional Theory simplifies 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. Our claims are substantiated by simulations of embedded ground and excited states (including charge transfer) of liquids, crystals, and layered systems. By suppressing the inter-subsystem self-interaction error inherent in the exchange–correlation functional, subsystem DFT yields substantially improved simulations compared to Kohn–Sham DFT at a fraction of the computational cost - achieving a dual saving: time to the researcher, and energy to our planet.

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