

Abstract Submitted
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A unified quantum mechanics embedding theory for materials and molecules¹ CHEN HUANG, Department of Physics, Princeton University, Princeton, New Jersey 08544, USA, MICHELE PAVONE, EMILY CARTER², Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544-5263, USA — It is essentially impossible to apply highly accurate quantum mechanics methods to large material samples, creating a need for a sophisticated embedding theory that can locally refine the accuracy of predicted properties. Here, we present a new ab-initio embedding theory that can treat different regions in the material with quantum mechanics methods of appropriately varying levels of accuracy in a seamless way. We first remove the non-uniqueness of embedding potential definitions that exists in most previous embedding theories by introducing a physical constraint that all regions share a common embedding (interaction) potential. We then introduce a key step to achieve seamless embedding: reformulating the system’s total energy solely in terms of the embedding potential, i.e., we construct a potential-functional embedding theory (PFET). We demonstrate how to efficiently solve PFET for molecules and materials and give an outlook for how to perform seamless “multi-physics” material simulations with PFET.

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