Embedding as a new perspective on electronic structure theory

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The concept of embedding is at the heart of electronic structure theory: even Hartree-Fock theory works by considering the quantum mechanics of a single electron embedded in an effective potential that approximately describes interactions with the environment. Embedding has been used very widely in theoretical chemistry, and common examples of embedding of one kind or another include QM/MM calculations, polarisable continuum and use of effective core potentials. Here I will discuss the use of embedding for high-accuracy description of condensed matter, and, more generally as a framework for developing new electronic structure methods.

The work on condensed-matter systems concentrates on various ways to incorporate many-body effects into truncated many-body expansions, and can be used, for example, in the study of organic crystals.

In more general terms, embedding will be explored as an alternative to inter-pair coupling (which led from the independent-electron pair approximation to coupled-cluster theory) and to higher excitation levels.