Site-occupation embedding theory for the treatment of strongly correlated systems

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Strongly correlated materials (like transition metal oxides) have attracted much attention over the years and remain one of the main central and challenging research topic, gathering chemists and physicists, theoreticians and experimentalists. Being able to understand and even predict the properties of such systems can shape the technologies of the future by the design of new nanodevices, with applications to energy conversion and electronic transport for solar cells, superconducting magnets generating strong magnetic fields, and colossal magnetoresistance materials for magnetic storage.

When it comes to describing strongly correlated materials or molecules, the standard low cost methods such as density functional theory usually fail. While more involved wavefunction-based approaches could in principle be applied, they remain out of reach due to the prohibitive computational cost. A natural and intuitive idea is to merge the two methods to build a new one that gathers all advantages: a low computational cost and good accuracy. From a mathematical point of view, such a combination is very similar to the so-called 'embedding approaches' which are becoming increasingly popular in quantum chemistry[1]. Over the last decade, there has been a clear increase in interest in embedding techniques, which focus only on a small part of a much larger system. One of the most difficult tasks is the incorporation of the nonlocal electron correlation effects induced by the rest of the system (often referred to as the environment). Providing an exact formulation of such a theory is far from trivial since the methods to be merged are written in completely different formalisms.

My thesis dealt with the development and practical implementation of a novel and in-principle-exact embedding approach which is referred to as site-occupation embedding theory (SOET)[2-4]. We first tested it on the Hubbard model, which is mostly used in condensed matter physics for describing strongly correlated materials. Although still in its early stages, promising results have been obtained within SOET and our theory could progress in any of the direction mentioned at the beginning of this abstract.

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