Molecular Physics Longuet-Higgins Early Career Researcher Prize 2017

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Winning article: Local density approximation in site-occupation embedding theory

When it comes to describe strongly correlated materials or molecules, the standard low cost methods, such as density functional theory (DFT), usually fail. While more involved wavefunction-based approaches could in principle be applied, they remain out of reach in terms of 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 become increasingly popular in quantum chemistry. Indeed, we are now in a situation where Moore's law reaches its limit, thus forcing us to rethink computational modelling and, in particular, to lend weight to the development of low-cost embedding approaches for the modelling of larger systems.

Providing an exact formulation of the hybrid theory is far from trivial since the methods to be merged are written in completely different formalisms. My paper deals with the development and practical implementation of a novel embedding approach which is referred to as *site-occupation embedding theory* (SOET). The in-principle-exact formulation of SOET is important and helpful to understand what is usually missing in the popular embedding approaches, and therefore paves the way towards the development of new efficient embedding schemes.

Still in its early stages, SOET is a promising method for the modelling of strongly correlated systems. Such systems, 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. SOET could progress in any of these directions.