Does coupled cluster theory work for metals?

Routine application of electronic structure theories has become almost ubiquitous in materials design and applied condensed matter physics. However, for experimentalists and theoreticians alike, there is a desire for a more reliable tool than density functional theory as and when needs arise. This is especially true for situations in which the band gap of a system is small, or closes, and the electronic structure becomes metallic.

There is great potential for coupled cluster theory to provide the next generation of theories for these fields, but we need to check that the vanishing gap does not cause a problem for our methods. We have long been aware, for instance, that perturbative methods diverge when treating a Coulombic metal.

I will discuss how a series of simple simulations of homogeneous electron gas models can numerically determine whether a wave function method is suitable for the treatment of metallic systems. It is our hope that this analysis will aid in the development of new electronic structure techniques.

This talk will describe work published in the following papers.

James J. Shepherd and Andreas Grüneis
Phys. Rev. Lett. 110, 226401 (2013)

James J. Shepherd, Thomas M. Henderson and Gustavo E. Scuseria
Phys. Rev. Lett. 112, 133002 (2014)

James J. Shepherd, Thomas. M. Henderson and Gustavo E. Scuseria
J. Chem. Phys. 140, 124102 (2014)