Versatility and Interpretability in Electron Propagator Theory

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2014 Sanibel Symposium

Abstract

The versatility of electron propagator concepts in chemistry is revealed by their application to a variety of problems that animate experimental investigation. This methodology underlies highly efficient algorithms for the calculation of electron binding energies of large molecules, including cases where the effects of correlation are qualitatively important. Generalizations to non–electronic binding energies have shown considerable promise with the use of simple self–energy approximations. Self–energies that been extensively applied to isolated molecules may be used to calculate electric currents in molecular wires and electron binding energies of solvated species. In all of these applications, one–particle concepts that incorporate the effects of correlation yield clear, generalizable interpretations that may guide the design of subsequent experiments.