# Prediction and Interpretation with Ab Initio Electron Propagator Theory

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Quantum chemistry, or molecular electronic structure theory, has had two chief missions in the recent history of chemistry. First, it has sought to provide accurate means of calculating molecular properties and its success in this respect has made it an important component in the education of computational chemists. The second mission, providing qualitative insight into chemical bonding, amplifies the ability of chemists to conceive of new patterns of structure, energetics and reactivity and to communicate their ideas to colleagues and students alike. Molecular orbital theory has broadly influenced quantum chemistry in both respects, but attempts to improve its quantitative, predictive capabilities often sacrifice the transparency of its interpretive attributes. Electron propagator theory provides a rigorous means to calculating molecular properties that retains many of the interpretive advantages of molecular orbital concepts. One-electron equations with a nonlocal, correlation potential known as the self-energy yield electron binding energies and Dyson orbitals, which in turn may be used to evaluate other properties. The resulting orbital picture of electronic structure is easily interpretable and, through systematic improvements to the self-energy, may be used to generate accurate predictions of spectroscopic experiments. Efficient implementations of these ideas enable applications to a variety of systems of experimental interest, including nucleotide fragments, fullerenes and anions with unusual electronic structure.