Electronic Structure Methods for Large Molecules and Novel Applications in Nanoscience

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The development of accurate and broadly applicable models for large molecules continues to be a major challenge in quantum chemistry. Hybrid models (where the central region and the surrounding region are partitioned and treated with two different levels of theory) offer a promising avenue for modeling large systems. We are presently developing a hierarchy of embedded cluster methods, where the treatment ranges from simple point charge electrostatic embedding to including the effects of charge transfer across regional boundaries to more complex treatments involving multiple fragments and interactions. We will qualitatively describe our new models and present results from novel applications such as dye-sensitized solar cells and peptide conformations.