Combined Quantum Monte Carlo-Effective Fragment Molecular Orbital Method

F. Zahariev and **M. S. Gordon**

Iowa State University

A novel combined Quantum Monte Carlo (QMC) Effective Fragment Molecular Orbital (EFMO) method is presented. The QMC-EFMO method inherits the advantages of the two combined approaches: the high accuracy of the QMC computational results and the favorable computational scaling due to the EFMO fragmentation of large systems. The combined QMC-EFMO method is illustrated on several water-containing clusters and a mesoporous silica nanocluster (MSN) model.