Some Recent Developments in Quantum Chemical Methods for Treating Electron Correlations

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Abstract:
An adequate description of electron correlation is vital to a successful electronic structure method. At the same time, a complete description of electron correlation remains largely out of reach for routine computational studies of interesting problems in molecular chemistry due to computational requirements. Therefore some tradeoff between accuracy and computational feasibility is required. I will discuss some recent developments from my group that show promise for practical applications to chemical problems. The first focus of the talk will be what under what conditions modern density functional theory (DFT) methods perform well, with quantitative assessments of "how well?". The second focus of the talk is a discussion of wavefunction methods that can tractably supplement DFT methods for complex problems where delocalization errors or strong correlation effects are at play. I plan to present some interesting examples of such cases.