

Progressing to Full Configuration Interaction

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Finding exact wave functions for electrons is famously intractable. In recent years we have seen new approximations that push back the boundaries of the full configuration interaction (FCI) limit, with considerable success. These methods have reduced the computational cost of FCI by orders of magnitude and maintained systematic improvability, allowing charting of new territory with benchmark-level accuracy. At the same time, however, the exponentially-scaling cost of FCI inevitably halts these advances for larger systems. The Zimmerman group has therefore introduced incremental FCI (iFCI), which seeks to approach the FCI limit at polynomial cost. This talk will discuss how the method works, recent progress in iFCI, and how fast CI solvers are instrumental to maintaining tractability. Application of iFCI to strongly correlated transition metal complexes with over 100 electrons will demonstrate the scope of its applicability.