

X Workshop on Novel Methods for Electronic Structure Calculations

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Methods for Strong Electron Correlation

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Quantum Chemistry is a mature field. Progress in the last 50 years has been fantastic. The weak electron correlation problem has been conquered by coupled cluster theory, but strong correlation remains pervasive and problematic. Many practical applications are hindered by this obstacle. Of course, it is not surprising that after almost 100 years of Schrodinger equation, only the most difficult problems are left. In the past decade, my research group has focused on strong correlation, and in this talk, I will discuss our recent efforts to tackle it. Our current approach centers around the hope that a noncanonical duality may convert strongly correlated electrons into weakly correlated ones. Many-body string operators, whose matrix elements can be obtained with polynomial cost, play a central role in our approach. I will present proof of principle applications to model systems where the interaction strength can be tuned.