Tensor product states for more compact electronic state descriptions

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If current activity provides a reasonable outlook over the next several years, one might safely assume that developing ways to model strongly correlated systems will become increasingly important to the field, likely using techniques involving machine learning, embedding, tensor networks, and quantum computing. In this talk, I will describe our group's recent efforts to use tensor product states for more compact descriptions of electronic states. In this approach, we use eigenstates of local reduced density matrices as a way to construct a basis in which the exact global state has increased sparsity. This increased (but unstructured) sparsity can be exploited by selected CI approaches which use the Hamiltonian to identify important configurations, defining a method we refer to as tensor product selected CI (TPSCI). Numerical results will be presented which highlight the faster convergence to FCI compared to methods based on Slater determinants.