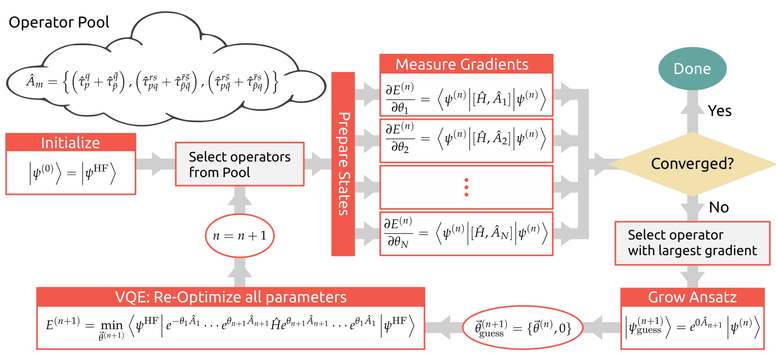
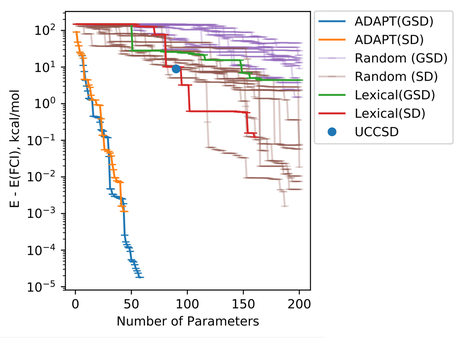
mayhall group | Virginia Tech

Critical problems in all areas of chemistry benefit from a microscopic understanding of structure and mechanism. Computational chemistry provides an exceptionally detail-rich glance into the inner workings of molecular events. Our research activities focus primarily on the development of novel quantum chemistry methods and the application of these methods to investigate the chemical foundations of renewable energy sources and quantum technologies.

quantum algorithms

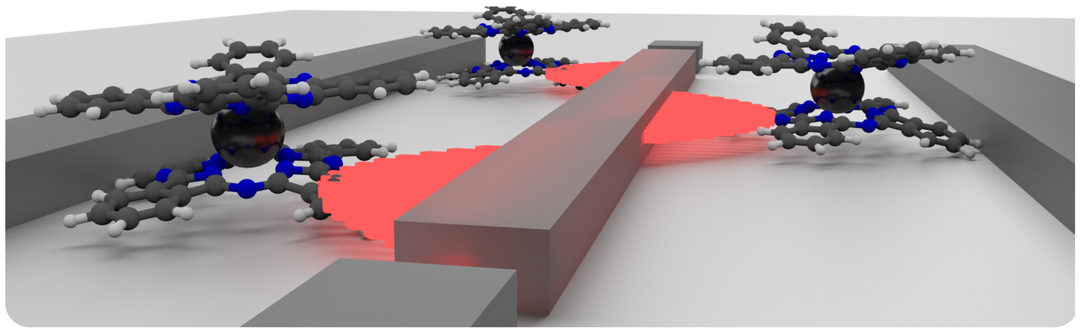
Quantum computing offers the exciting possibility of side-stepping the exponential scaling associated with simulating chemistry systems at the quantum level. However, in order to achieve this, new algorithms which can run on quantum devices need to be developed and tested. We are working on developing adaptive quantum algorithms, specifically focused on realizing improved molecular simulations on quantum hardware.





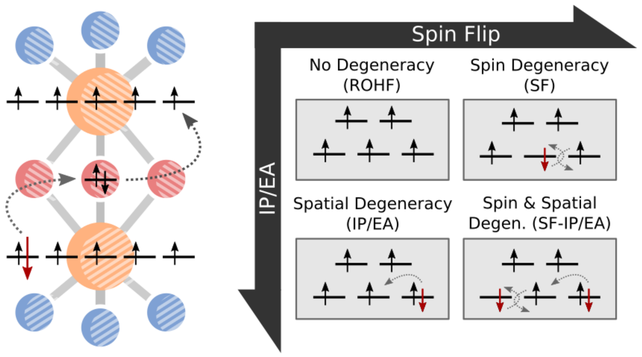
molecular qubit simulation

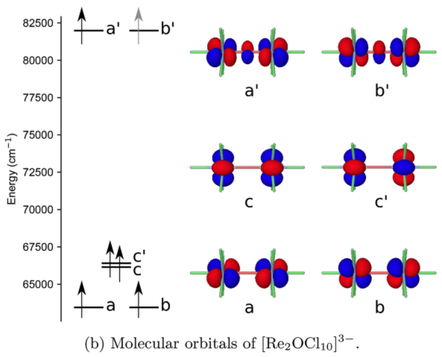
Unlike in traditional (classical) computing where the devices are largely determined by material properties, the small sizes of quantum bits, means that the device performance will be determined by both material and molecular properties. We are interested in developing methods and running simulations for understanding which chemical characteristics (and to what extent) affect the performance of single molecule magnets for quantum information purposes.



fock space CI methods

Entangled electrons in molecular magnets, strongly correlated transition metal catalysts, many of our most important problems are not easily modelled with conventional quantum chemistry. We have an ongoing interest in the use of the spin-flip framework (pioneered by Anna Krylov at USC) for describing several types of strongly correlated systems within a single reference formalism.

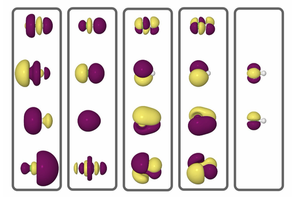


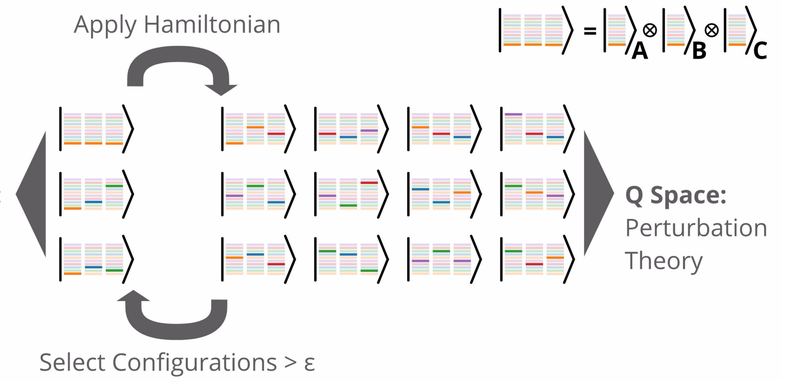


(b) Molecular orbitals of $[Re_2OCl_{10}]^{3-}$.

tensor product approximations

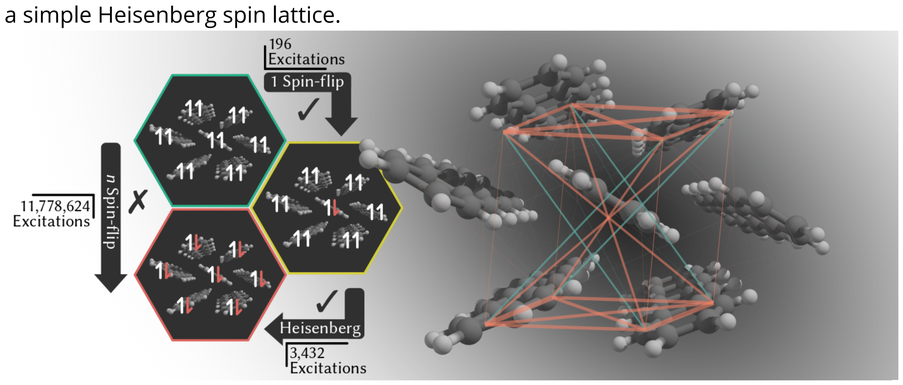
We work on developing new tools to efficiently model systems containing strongly correlated electrons. One approach to this problem is to consider tensor decompositions as a way to decrease the complexity of representing strongly correlated systems. We've recently designed a framework for simulating structured molecules with a so-called "Tucker Decomposition". This particular decomposition hasn't seen much use due to the fact that it still scales exponentially with system size - similar to FCI. However, we've leveraged the techniques from selected Configuration Interaction to develop numerically accurate approximations to the core tensor. Many new directions from this work are possible.





molecular material excitations

We work on developing computational techniques to understand the detailed structure and mechanisms which characterize such photoactive molecular materials, in an effort to design new materials with tailored photophysics. In one recent approach, we have used single-excitation wavefunctions (low-cost) to characterize multiexcitons in organic chromophore clusters. This approach works by establishing a one-to-one relationship between the elements of a Bloch-effective Hamiltonian obtained from one spin-flip calculations and a simple Heisenberg spin lattice.



large molecule strategies

Fragment-based and embedding methods are simple approaches to reduce the cost of electronic structure theory calculations. However, often these methods rely more on heuristics than well-controlled approximations, and thus error management is more of a problem. We have had an interest in these fragment-based approaches for some time, and more recently we have also developed improvements to the projection based embedding approach.