Abstract: High-Accuracy Transition Metal Organometallic Database of Thermodynamic Properties

This proposal continues an XSEDE startup allocation, the goal of which is to develop a new database for inorganic and organometallic species containing first-row transition metals. This database will include thermodynamic & electronic properties, geometry optimization steps,
molecular orbitals, and orbital energies at various levels of theory and basis set size. This database will provide the theoretical and computational community a database of high accuracy thermodynamic & electronic properties that covers the most experimentally relevant structural motifs. Thereby providing a much-needed bridge between the experimental and computational community in this area. The primary use of this database is to utilize the data in machine learning applications, the study of thermochemical and physical properties of transition metal containing species, and to provide a publicly available resource to advance the development of new and improved theory and computational approaches to transition metal chemistry.
We have chosen to focus on first-row transition metals to provide the most useful and accurate data possible since heavier metals often require relativistic effects. The ligands chosen for each metal center represent those found most frequently within the current literature scope. We have similarly chosen to focus on the most common spin and oxidation states of the first-row transition metals. 105 individual structures have been selected for each of the ten 3d transition metals.
All calculations performed in the development of this database will have chemical properties compiled into the database labeled with the details of the computation performed. To enable facile use of the database in the broader theoretical & computational communities. the structure and layout of this database will be modeled after the new database architecture developed as part of the Molecular Sciences Software Institute (MolSSI) objectives. The data collected in this database will include thermodynamic properties (e.g., internal energy, enthalpy, and Gibb's free energy), as well as properties derived from the electronic calculations (e.g., HOMO/LUMO energies, dipole moment, ionization potential). Thermodynamic properties will be obtained via composite methods, while the electronic properties will be collected from each calculation at the levels of theory and basis set sizes that are required for our chosen composite method.