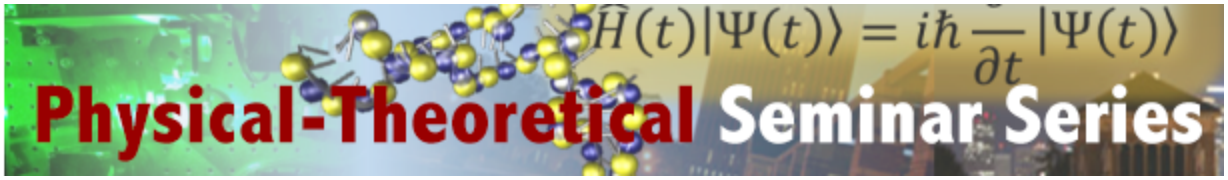

Friday, April 30, 2018, 12:00 pm
Seaver Science Library, Room 150
SSC Auditorium next to the library

Professor Laura Gagliardi

Department of Chemistry
University of Minnesota

Electronically Excited States and Metal Containing Systems are a Challenge for Modern Quantum Chemistry

I will report our latest developments of multireference methods with special focus on multiconfiguration pair-density functional theory (MC-PDFT) and its application to understanding the properties and reactivity of electronically excited states and transition metal-containing systems. MC-PDFT [1] combines mutireference wave functions and density functional theory methods to treat strongly correlated systems. I will illustrate examples of multireference systems, including single molecule magnets containing actinides [2] and organic radicals [3]. Finally I will discuss our latest extension of multireference methods to complex systems using density matrix embedding theory.[4]

[1] L. Gagliardi, D. G. Truhlar, G. Li Manni, R. K. Carlson, C. E. Hoyer, and J. Lucas Bao, Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems, Acc. Chem. Res., **50, 2017**, pp 66–73

[2] M. Spivak, K. D. Vogiatzis, C. J. Cramer, C. de Graaf, and L. Gagliardi, Quantum Chemical Characterization of Single Molecule Magnets Based on Uranium, J. Phys. Chem. A, **8**, **2017** 1726-1733

[3] S. J. Stoneburner, J. Shen, A. O. Ajala, P. Piecuch, D. G. Truhlar, and L. Gagliardi, Systematic Design Of Active Spaces For Multi-Reference Calculations Of Singlet– Triplet Gaps Of Organic Diradicals, With Benchmarks Against Doubly Electron- Attached Coupled-Cluster Data, J. Chem. Phys., **147, 2017** p 164120

[4] H. Q. Pham, V. Bernales, and L. Gagliardi Can Density Matrix Embedding Theory with the Complete Activate Space Self-Consistent Field Solver Describe Single and Double Bond Breaking in Molecular Systems? J. Chem. Theory and Comp. DOI:10.1021/acs.jctc.7b01248, **2018**

Hosted by Professor Anna Krylov

The scientific community is invited

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