Modern Quantum-Chemical Methods for Complex Chemistry

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In this talk I will demonstrate how we exploit concepts from quantum information theory to automate the crucial active orbital space selection in multi-configurational calculations.[1] The main quantities required for this procedure, the orbital entanglement measures, are derived from reduced one- and two-orbital density matrices and are directly connected to static correlation. Our automated selection protocol is implemented in the graphical user interface autoCAS.[2]
I will then discuss further applications of these measures in inorganic chemistry.
In the last part of my talk I will shift gears slightly and introduce the main topic of my postdoctoral research project at UC Berkeley: electrocatalysis on metal clusters with coupling to an electron reservoir.

[1] C.J. Stein, M. Reiher, *JCTC*, **2016**, *12*, 1760.
[2] www.scine.ethz.ch/autocas