Autonomous Active Space Calculations through AutoCAS

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In order to describe strongly correlated systems correctly, the choice of an active space imposes one of the greatest problems in multi-configurational quantum chemistry. In the AutoCAS algorithm, concepts from quantum information theory are exploited in order to automatically and consistently select orbitals for an active space. We present our `Python`-based AutoCAS [1, 2, 3, 4] module, which can be customized and employed in existing workflows to streamline multi-configurational calculations in a black-box manner. Due to the black-box-like selection of active spaces, post-active space methods like Tailored Coupled Cluster [5, 6, 7] or second order perturbation theory [8] can be routinely applied to recover dynamic correlation. Furthermore, in the AutoRXN workflow [9], a workflow for the exploration of chemical reaction networks, we automatically validated CCSD(T) energies with potential multi-reference character through AutoCAS.

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