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Automated Active Space Selection Using Large Language Models

The Multi-Reference Electronic Structure Theory involves choosing an active space with knowledge of the subspace's spatial and energetic information within the Hilbert space of a molecular electronic Hamiltonian that exhibits strong correlation. This process can be automated with the help of an AI assistant. This paper presents such an assistant that utilizes tools like the Approximate Pair Coefficient (APC) and the Atomic Valence Active Space (AVAS). Additionally, the assistant has a fine-tuned Large Language Model that can determine the active space required for a given molecular state with informed decisions.

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