

Quantitative Description of Strongly Correlated Materials by Combining Downfolding Techniques and Tensor Networks

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We present a high-accuracy procedure for electronic structure calculations of strongly correlated materials. To address limitations in current electronic structure methods, we employ density functional theory in combination with the constrained random phase approximation to construct an effective multi-band Hubbard model, which is subsequently solved using tensor networks. Our work focuses on one-dimensional and quasi-one-dimensional materials, for which we employ the machinery of matrix product states. We apply this framework to the conjugated polymers trans-polyacetylene and polythiophene, as well as the quasi-one-dimensional charge-transfer insulator Sr_2CuO_3 . The predicted band gaps show quantitative agreement with state-of-the-art computational techniques and experimental measurements. Beyond band gaps, tensor networks provide access to a wide range of physically relevant properties, including spin magnetization and various excitation energies. Their flexibility supports the implementation of complex Hamiltonians with longer-range interactions, while the bond dimension enables systematic control over accuracy. Furthermore, the computational cost scales efficiently with system size, demonstrating the framework's scalability.