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High-performance spectrum calculation of 3d transition metals in oxide compounds

In the early 20th century, quantum mechanics revolutionized material studies, leading to the invention of the transistor, the key component of modern day technologies. To sustain technological advancements, innovations in new materials are needed, with 3d transition elements showing immense potential. A common method in the study of the electronic structure of these elements is X-ray Absorption Spectroscopy (XAS). This method generates spectra that show how a material absorbs X-rays at various energy levels. However, interpreting experimental spectra can be challenging due to observed unexplainable features. Therefore, theoretical methods are necessary to extract information and analyze the spectra. In this work, we present a theoretical approach to interpret XAS spectra. First, we construct real and symmetric Hamiltonian matrices representing 3d transition elements with atomic numbers 21 to 29, with dimensions ranging from 50 thousand to 16 billion. Next, we use the SLEPc library to determine the ground state eigenvalues of specific Hamiltonians. Following this, we initialize the Lanczos iterative method with an expansion of the ground state eigenvalue to calculate the necessary eigenpairs for spectrum plotting. These eigenpairs represent the energy levels of the material when exposed to X-ray beams. Finally, we compare our theoretical results with experimental data, demonstrating strong agreement. Our findings underscore the effectiveness of our theoretical method in interpreting XAS spectra and advancing the study of 3d transition elements.