MAHTA ABDOLLAHZADEHZARE, University of Saskatchewan

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

In the early 20th century, the principles of quantum mechanics revolutionized the study of materials, leading to the invention of the transistor, the key component of modern day technologies. To sustain advancements in technology, innovations in the discovery of new materials are needed. One family of elements with immense potential in creating new functional materials is the 3d transition elements, especially in the form of oxide compounds. A common method in the study of the electronic structure of such compounds is X-ray Absorption Spectroscopy (XAS). This method yields spectra of the energy-dependent absorption which, for energies near atomic resonances, contains detailed electronic and magnetic information about the materials. However, interpreting experimental spectra can be challenging due to complicated lineshapes arising from quantum many-body interactions. Therefore, theoretical methods are often necessary to extract information and analyze the spectra. This study focuses on quantum double cluster models to simulate spectra, in particular constructing real, symmetric Hamiltonian matrices for oxide compounds containing 3d transition elements with atomic numbers 21 to 29. We employ the SLEPc library to determine the ground state eigenvalues of specific Hamiltonians, and utilize the Lanczos iterative method to calculate the XAS spectra. Our results reveal the range of necessity of this double cluster model over the series of 3d elements via the extracted covalency from the ground state wavefunction and the differences of XAS spectra compared to simpler single cluster models.