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Quasipartice Band Structure and Optical Properties of α-MnO₂ : A Beyond Density Functional Theory Investigation

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The quasi-particle band structure and the optical properties of spin polarized bulk α-MnO₂ have been investigated by means of many body perturbation theory within an ab initio framework. As a starting point the electronic band structure obtained from Density Functional Theory with Hubbard correction (DFT+U, U = 2.4 eV) approach show that bulk α-MnO₂ is a semiconductor with a band gap of 1.284 eV. Quasi-particle band structure within the G₀W₀ level of approximation yields a band gap of 2.38 eV. Moreover, for the optical properties calculations, two particle excitations have been included through solving the Bethe-Salpeter equations (BSE) for the electron-hole pair correlation function. The peaks in the optical spectra are discussed based on the transitions within the computed band structure. From our results, the structure exhibits a strong optical absorption in the visible region along all the crystallographic directions. The optical anisotropy in this material is analyzed by means of dielectric function as well as the optical absorption coefficients along different principal axes. For instance, in the visible region, the calculated values for the highest absorption coefficients are 3.69×10^{−5}cm^{−1} along [100 and 010] and 6.32×10^{−5}cm^{−1} along [001] components. This clearly indicates the optical anisotropic behaviour in α-MnO₂. The optical absorption spectrum predicts a strong bound exciton that lies below the calculated quasi-particle band gap with binding energy of 0.65 eV in the bulk α-MnO₂.

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