# On the neglect of on-site Coulomb interactions on oxygen-ions in transition metal oxides described by multiband d-p model

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The electronic structure of transition metal oxides is frequently investigated using the multiband $d-p$ models, as in cuprates [1], ruthenates [2], and iridates [3]. On the example of $TiO_4$ layer we study the electronic structure within the multiband $d-p$ model. In agreement with experiment (for $Sr_2TiO_4$) we find that the studied system is predicted to be a robust nonmagnetic insulator. As expected, $d-p$ hybridization strongly redistributes electrons and leads to Ti ions between $d^1$ and $d^2$ ionic configurations. A realistic treatment of electronic structure requires one to introduce non-zero Coulomb local interactions at $2p$ oxygen orbitals [1-3]. We show that a simplified treatment which neglects Coulomb interactions on oxygen ions does not lead to serious problems in predictions of the electronic structure provided the Coulomb interactions at titanium ions and charge-transfer gap are suitably renormalized (so they become entirely different from those used in the microscopic $d-p$ model).

**References:**

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