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Improving the Conductivity of TiO_2 for Reducing Contact Resistivity with Silicon: A First-Principles Study and Experimental Demonstation

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Abstract

Transition metal oxides (TMOs) have been extensively explored as carrier-selective contacts for crystalline silicon (c-Si) solar cells as a replacement for the heavily doped silicon contact. Recently reported high efficiency c-Si solar cells, such as MoO_3-based 23.5%,[1] and TiO_x/LiF_x-based 23%,[2] silicon heterojunction solar cells show the potential of TMOs as efficient, low-cost carrier-selective contact. TiO_2 has a high optical bangap of > 3 eV and exhibits excellent surface passivation on silicon. A LiF layer sandwiched between c-Si and TiO_2 film improved electron-selective passivation and interfacial contact resistivity of ~20 mΩ cm^{-2}, where first-principles density functional theory (DFT) calculations showed F-doping and the creation of additional defect states close to the conduction band of TiO_2.[3] Such defect states helped increasing the conductivity of TiO_2, crucial to reducing the contact resistivity with c-Si and efficiency of the solar cells. In this work we have extended this work and additional DFT calculations are conducted to reveal the most suitable defects/dopants to improve the conductance of TiO_2 films. Extrinsic interstitial and substitutional defects are considered in anatase. The defect formation energies are calculated followed by electronic density of states to understand the impact of the defects for electron selectivity with the c-Si. For examples, as shown in Figure 1, interstitially Al-doping creates additional defect states close to the conduction band of TiO_2 which could lower the contact resistivity with n-type c-Si. In addition to the electrical properties, also the optical properties are investigated as the addition of dopants can reduce the optical bandgap.

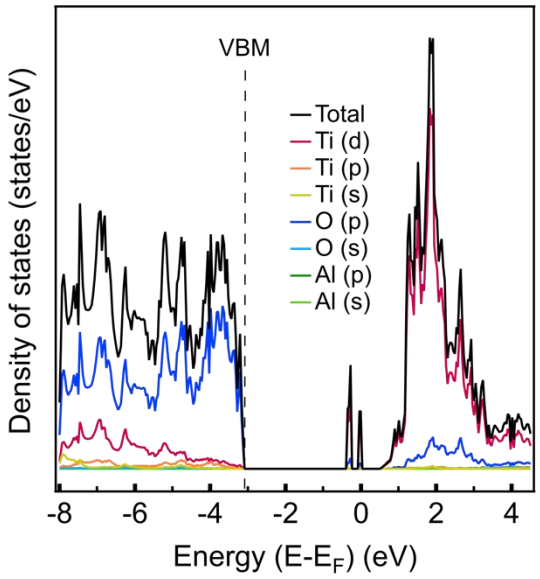

Figure 1. Calculated electron density of states of interstitial Al-doped anatase TiO_2.

References

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2. Bullock *et al.*, Adv. Energy Mater., 2019, 9, 1803367
3. Jian *et al*., ACS Nano, 2019, 13, 6356-6362