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| Title | An experimental and first-principles study of the effect of B/N doping in TiO2 thin films for visible light photo-catalysis | | |
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| Abstract |  |
| Thin films of TiO2 and boron–nitrogen (B/N) co-doped TiO2 on glass substrates have been prepared by a simple sol–gel dip coating route. Titanium (IV) isopropoxide, boric acid and urea have been used as titanium, boron and nitrogen sources, respectively. The films were characterized by X-ray diffraction, X-ray photo-electron spectroscopy, scanning electron microscopy, Raman spectroscopy and UV–vis spectroscopy. The TiO2 thin films with co-doping of different B/N atomic ratios (0.27–20.89) showed better photo-catalytic degradation ability of methylene blue compared to that of bare-TiO2 under visible light. The TiO2 film doped with the highest atomic concentration of N showed repeatedly the best photo-catalytic performance. The high activity of co-doped TiO2 thin films toward organic degradation can be related to the stronger absorption observed in the UV–vis region, red shift in adsorption edges and surface acidity induced by B/N doping. Furthermore, several atomic models for B/N doping have been used to investigate the effect of doping on electronic structure and density of states of TiO2 through ab-initio density functional theory calculations. The computational study suggested a significant narrowing of the band gap due to the formation of midgap states and the shift of Fermi-level for the interstitial N model supporting the experimental results. | |