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Exploring N3 ruthenium dye adsorption onto ZnTiO 3 (101) and (110) surfaces for dye sensitized solar cell applications: Full computational study
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Abstract
TiO 2 and ZnO binary oxide films are extensively investigated as photo-anodes in dye-sensitized solar cells (DSSCs), due to their large surface area, high electron mobility and chemical stability features. ZnTiO 3 perovskite is investigated as a photoanode, with N3 ruthenium dye, to design a new DSSC. First principal calculations based on DFT methods have been carried out to study the adsorption process of the ruthenium dye onto ZnTiO 3 (101) and (110) surfaces. The energy levels of N3 dye are studied and compared to available experimental data. The calculated energy band gap for ZnTiO 3 is 3.10 eV, which is in good agreement with experimental data (3.18 eV). The N3 dye is chemisorbed on the perovskite surface, via its carboxylic groups (COOH) which link to the (101) surface and two monodentate (ME) ester modes in (110) with bidentate bridging (BB) adsorption mode. The calculated adsorption energy (−241.50 kcal/mol) for the resulting N3@ZnTiO 3 complex, is much higher than the values for N3@ZnO (−89.58 kcal/mol) and N3@TiO 2 (−146.90 kcal/mol). The high adsorption energy of N3 dye, onto the perovskite surfaces, shows the potential value to use perovskites in future DSSCs. © 2019 Elsevier Ltd

Author Keywords
Adsorption energy; DFT calculation; DSSC; N3@ZnTiO 3 complex; Perovskite

Index Keywords
Adsorption, Chemical stability, Design for testability, Energy gap, II-VI semiconductors, Oxide films, Perovskite, Ruthenium, Solar cells, Titanium dioxide, Zinc oxide; Adsorption energies, Adsorption process, Computational studies, DFT calculation, DSSC, First-principal calculations, High electron mobility, N3@ZnTiO3 complex; Dye-sensitized solar cells

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