

## Investigation of the electronic structures and photoelectrical properties of cyanoacrylic dye on ZnTiO<sub>3</sub> perovskite for dye-sensitized solar cells

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The aggregation of sensitizers on a semiconductor is crucial for determining the light-harvesting efficiency of dye sensitized solar cells (DSSCs). The interfacial properties of dyes adsorbed on a ZnTiO<sub>4</sub> film, such as adsorption configurations and adsorption energy, can impact the total amount of dye sensitizers that loads and the stability of a DSSC device.

In this work ZnTiO<sub>3</sub> perovskite was selected as a photoanode for DSSC. First principal calculation study based on the DFT

method has been used to study the adsorption energy of the Cyanoacrylic dye onto ZnTiO<sub>3</sub> (101) and (110) surfaces. The electronic structures and photoelectrical properties of cyanoacrylic at ZnTiO<sub>3</sub> complex are performed using the generalized gradient approximation approach (GGA-PBE), in order to treat the vend-wells interaction, DFT-D approach was applied in CASTEP code.

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