

## Electronic Supplementary Information (ESI): Supporting Figures

This ESI contains supplementary figures related to the computational details, structural analysis, and optical properties discussed in the main manuscript.

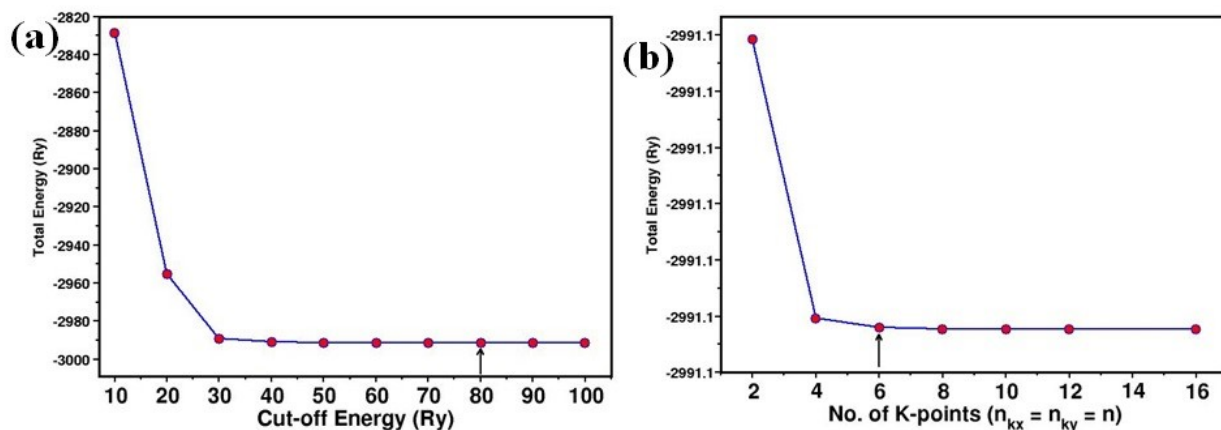


Figure S1: The plot of (a) Total Energy (Ry) against Kinetic Energy Cut-off (Ry) and (b) Total Energy (Ry) against number of k-Points along X and Y axes.

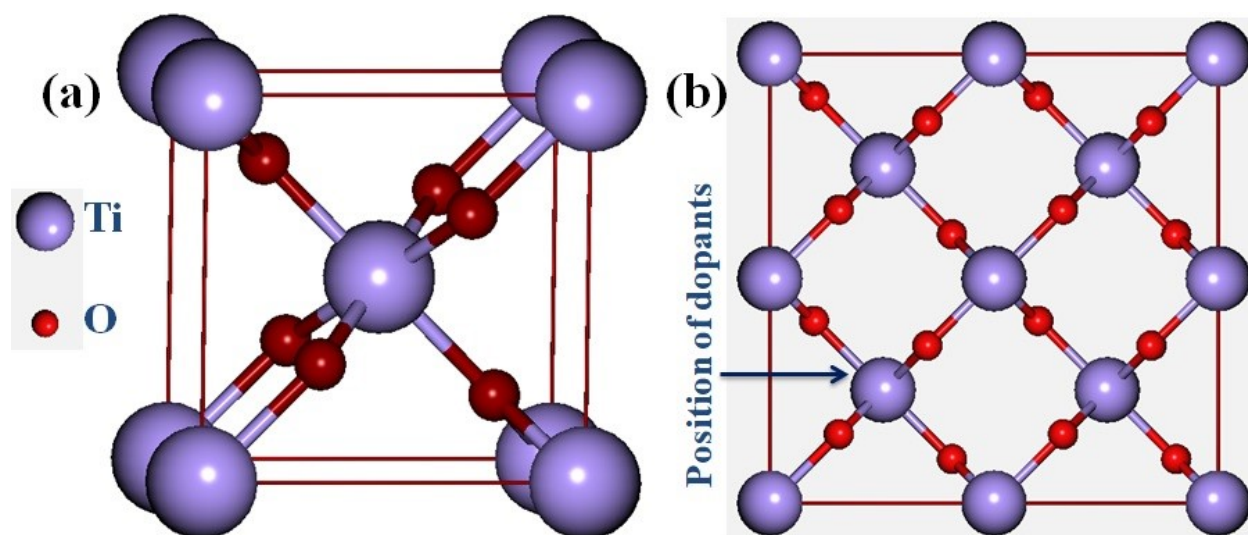


Figure S2: (a) Crystal structure of rutile  $\text{TiO}_2$  and (b) A lattice structure schematic of a  $2 \times 2 \times 2$  rutile  $\text{TiO}_2$  supercell.

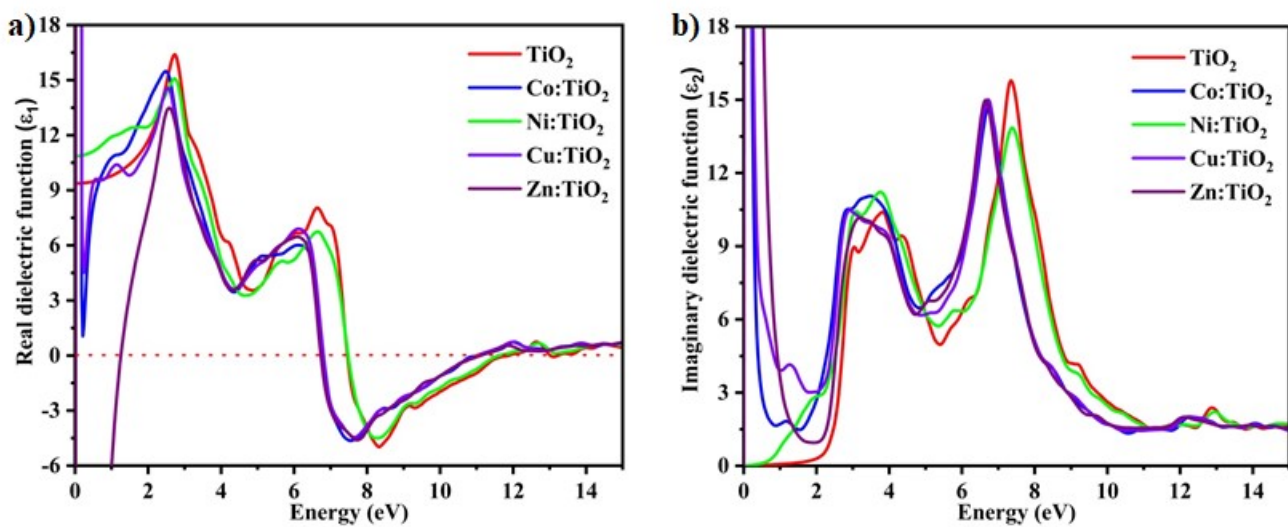


Figure S3 (a) Real part of dielectric function and (b) imaginary part of dielectric function as a function of photon energy the pure and doped TiO<sub>2</sub> at a concentration of 6.25%.