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A DFT Study on influence of solvent media on electronic, optical and vibrational properties of TiO2 Nanoparticle

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Density Functional Theory (DFT) is used to investigate the optical, electrical and vibrational properties of titanium dioxide nanoparticles (TiO2 NPs) by altering the solvent conditions from DI water to ethanol. From the theoretical calculations, it was observed that their HOMO-LOMO energy gaps are comparable with the experimental results. To study the electronic properties in detail, Koopmans' formulas are utilised to determine the binding energy per atom, energy gap, chemical potential, ionization potential, electron affinity, hardness and electrophilicity index. These parameters were calculated at the level of B3LYP with the LANL2DZ basis set using Gaussian 09 software. The IR and Ramman spectra for the proposed nanoparticles in different solvent conditions show the absorption and vibrational modes present in the system. This provides a clear indication of the solvent's effect on the physical and chemical properties of the TiO2 NPs.

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