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First Principles Optical Absorption Spectra of Organic Molecules Adsorbed on Titania Nanoparticles KOPINJOL BAISHYA, SERDAR OGUT[1], University of Illinois at Chicago, ERSEN METE, Balikesir University, OGUZ GULSEREN, Bilkent University, SINASI ELLIALTIOGLU, Middle East Technical University, Turkey — We present results from first principles computations on passivated rutile TiO_2 nanoparticles in both free-standing and dye-sensitized configurations to investigate the size dependence of their optical absorption spectra. The computations are performed using time-dependent density functional theory (TDDFT) as well as GW-Bethe-Salpeter-Equation (GWBSE) methods and compared with each other. We interpret the first principles spectra for free-standing TiO_2 nanoparticles within the framework of the classical Mie-Gans theory using the bulk dielectric function of TiO_2. We investigate the effects of the titania support on the absorption spectra of a particular set of perylene-diimide (PDI) derived dye molecules, namely brominated PDI ($Br_2C_{24}H_8N_2O_4$) and its glycine and aspartine derivatives.

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