Efficiency of Interfacial Charge Transfer Complex Between TiO_2 Nanoparticles and Caffeic Acid Against DNA Damage *In vitro*: Combinatorial Analysis

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Numerical calculations

The optical properties of ICT complex between TiO_2 NPs and CA were obtained by quantum chemical calculations based on Density Functional Theory (DFT) and Time-Dependent DF Theory (TD-DFT). The $[Ti_{18}O_{33}(OH)_6]$ cluster, derived from the bulk anatase TiO_2, was used as a model system for the calculations. The ground state geometry of $CA/[Ti_{18}O_{31}(OH)_8]$ complex was optimized using the B3LYP hybrid functional [1, 2], in combination with 6-31G(d,p) basis set [3]. Frequency calculations were carried out at the same level of the theory, and the absence of imaginary frequencies confirmed that all optimized structures are true minima. To preserve the crystal structure of anatase, the positions of titanium and oxygen atoms of the cluster have been frozen (kept fixed) during the optimization, while all atoms of the ligand molecules were allowed to relax. Also, the electronic excitation spectra were calculated at the same level of theory, within the TD-DFT formalism by taking into account the first 30 excitations . The solvent effect of water on the absorption spectra was included via SMD solvation model [4]. All calculations were performed with the use of Gaussian 09 suite of programs [5]. The convoluted electronic excitation spectra were obtained using GaussSum software [6].

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