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Article

Density functional theory study of optical and electronic properties of $(TiO_2)_{n=5,8,68}$ clusters for application in solar cells

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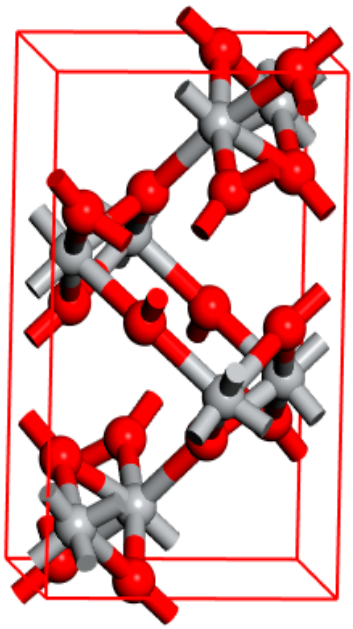
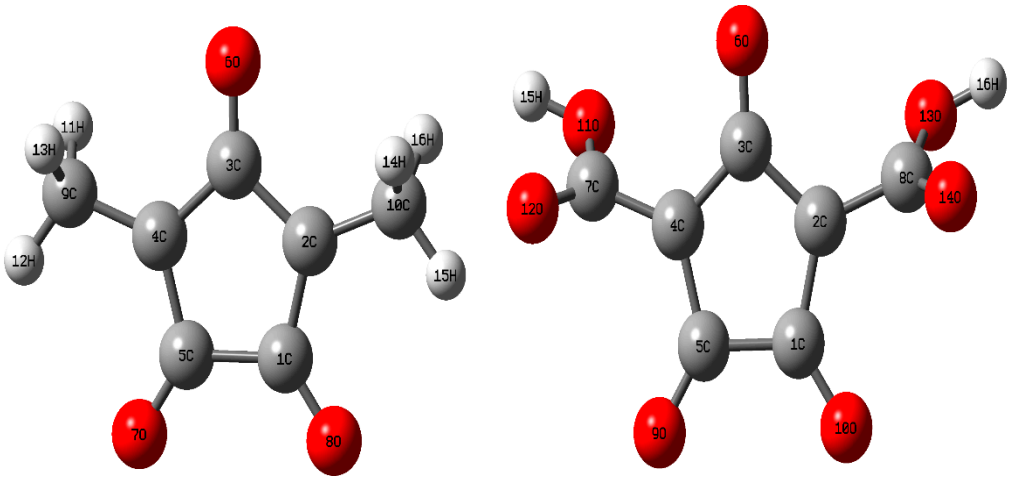


Figure 1. Crystallographic forms of TiO_2 brookite. The atoms are represented according to these colour schemes, grey balls are titanium atoms and red balls are oxygen atoms.



(a) **(b)**

Figure 2. a)-(b) (a) CR1 (b) CR2. The atoms are represented according to following colour scheme: grey balls represent titanium atoms, red balls represent oxygen atoms and white ball represent hydrogen atoms.

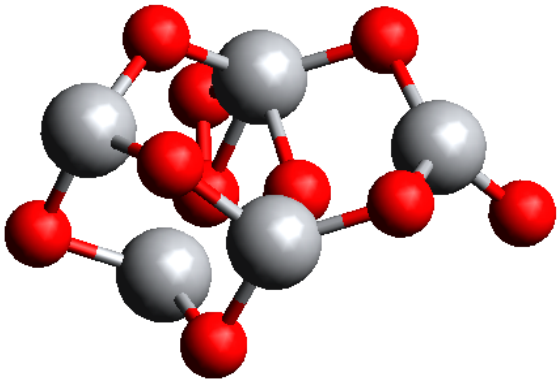


Figure 3. a). $(TiO_2)_5$ brookite cluster.

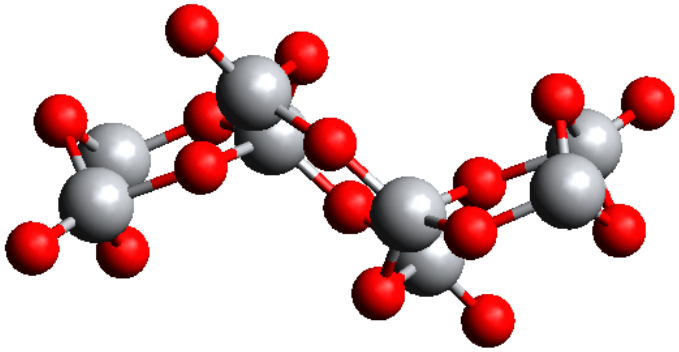


Figure 3. b). $(TiO_2)_8$ brookite cluster.

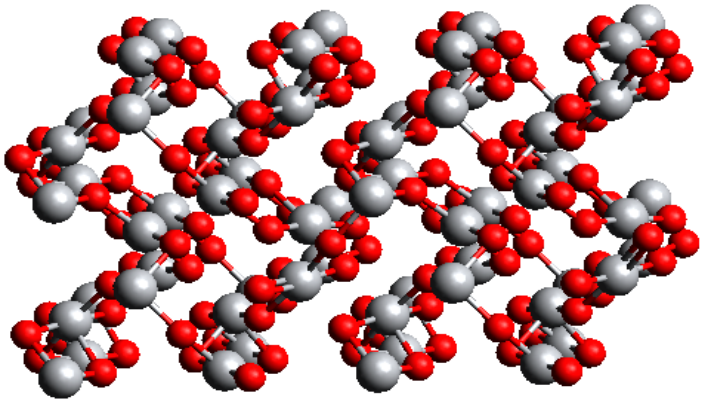
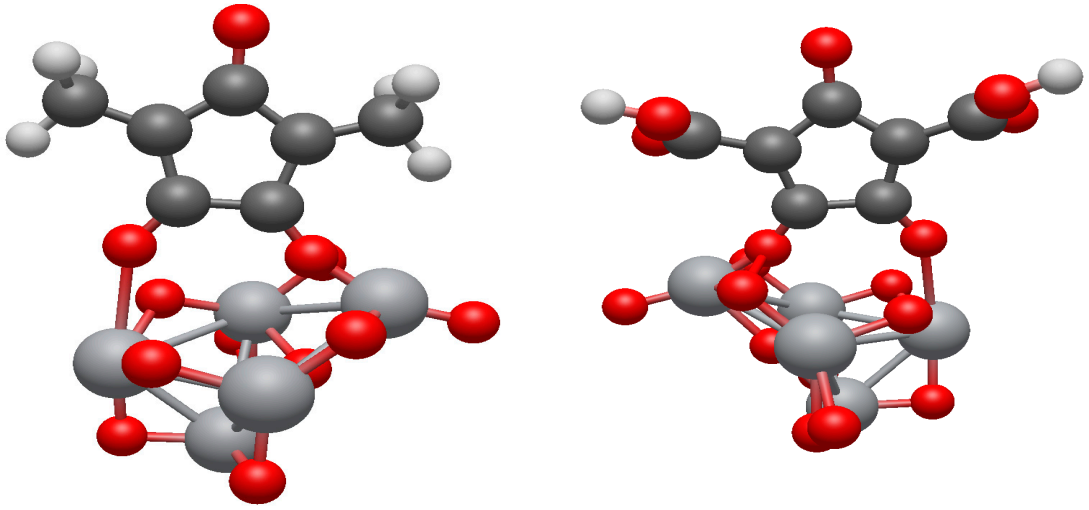
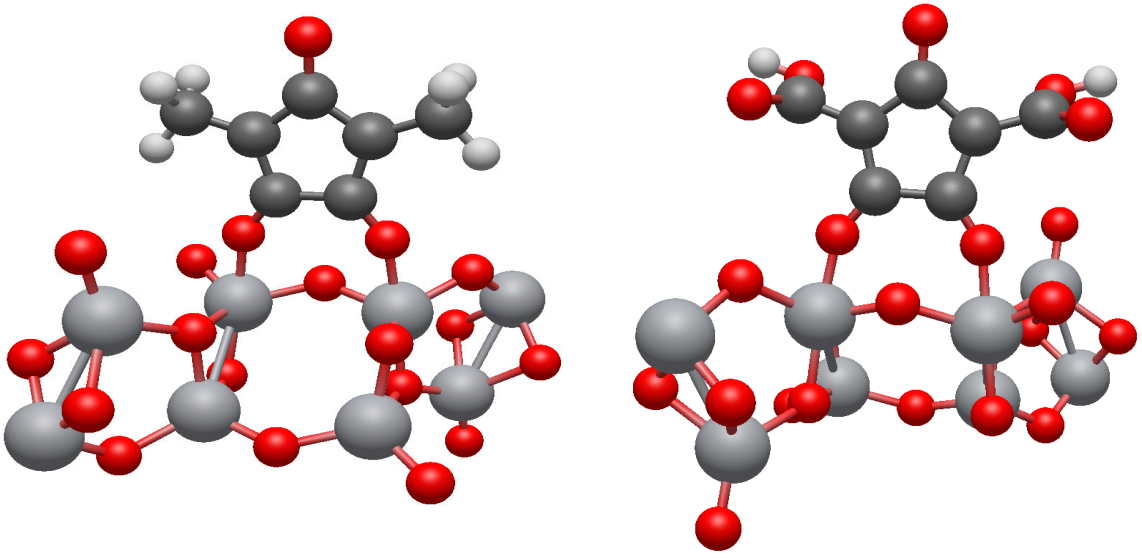


Figure 3. c). $(TiO_2)_{68}$ brookite cluster.



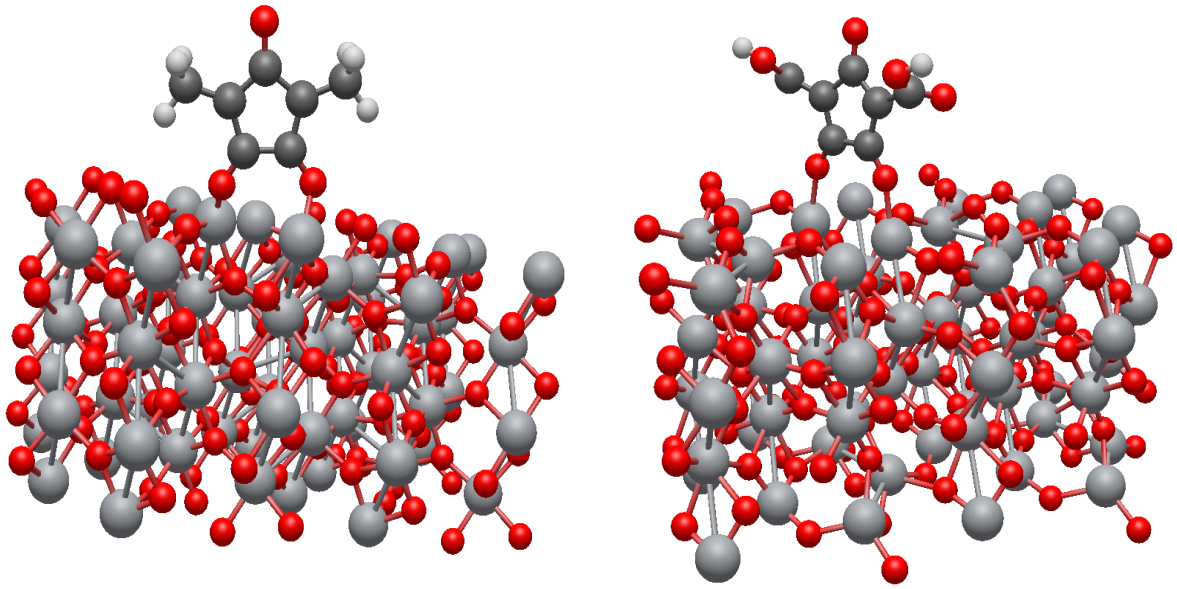
(a) **(b)**

Figure 4. Croconate dyes absorbed on $(TiO_2)_5$ nanocluster (a) CR1@ $(TiO_2)_5$ (b) CR2@ $(TiO_2)_5$.



(a) **(b)**

Figure 5. Croconate dyes absorbed on $(TiO_2)_8$ nanocluster (a) CR1@ $(TiO_2)_8$ (b) CR2@ $(TiO_2)_8$.



(a) **(b)**

Figure 6. Croconate dyes absorbed on $(TiO_2)_{68}$ nanoclusters (a) CR1@ $(TiO_2)_8$ (b) CR2@ $(TiO_2)_{68}$.

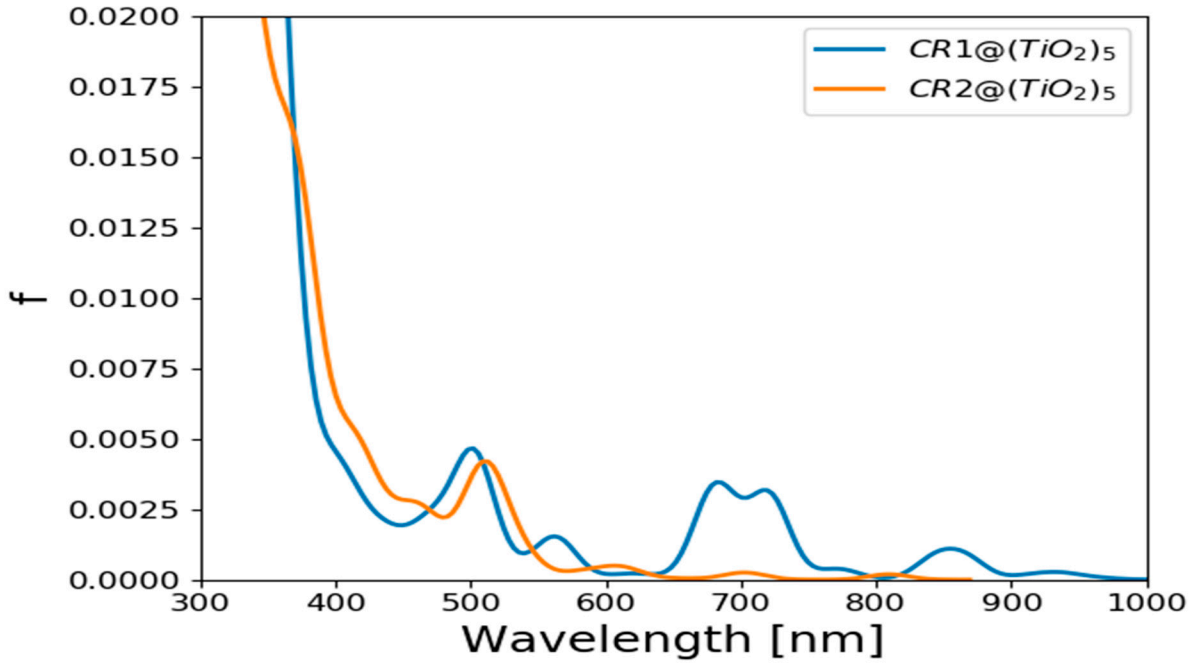


Figure 7. Expanded view of simulated UV-Vis spectrum of CR1 and CR2 absorbed on $(TiO_2)_5$ brookite cluster. The oscillator strengths were folded by Gaussians of emin=100, emax=1200nm width. The y-axis is "folded oscillator strength [1/nm].

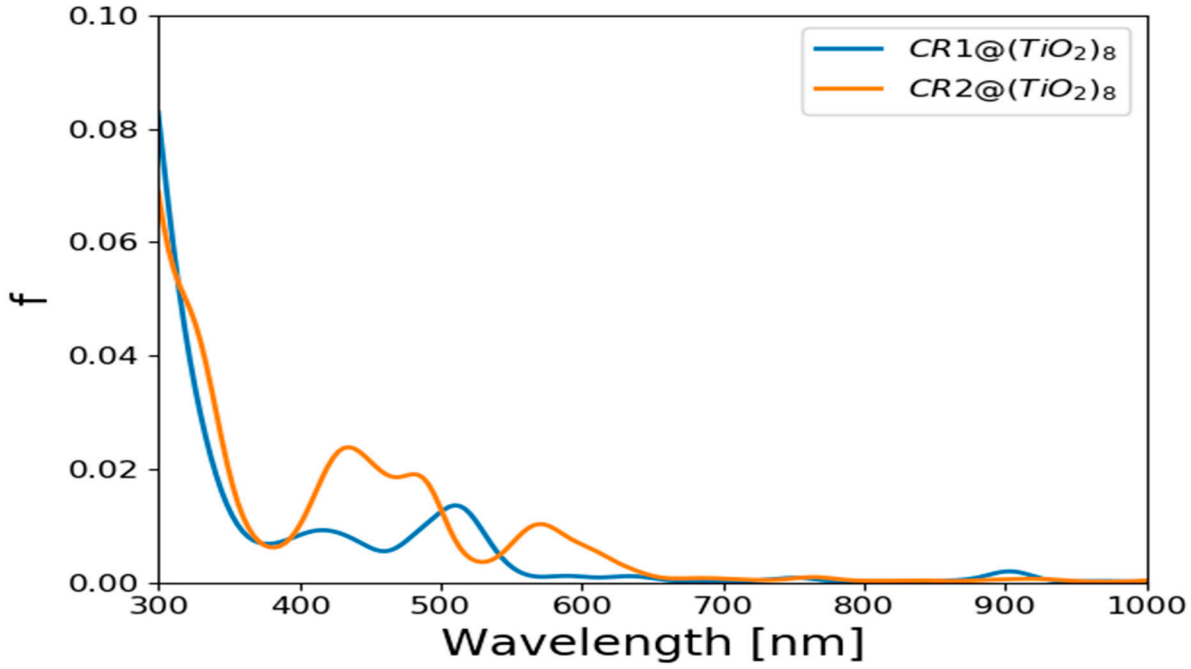


Figure 8. Expanded view of simulated UV/Vis absorption spectrum of CR1 and CR2 absorbed on $(TiO_2)_8$ brookite cluster. The oscillator strengths were folded by Gaussians of $e_{min} = 100$, $e_{max} = 1200$nm width. The y-axis is "folded oscillator strength [1/nm].