

## Free and Encapsulated (TiO<sub>2</sub>)<sub>2</sub> Dimers into Carbon Nanotubes

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**Abstract :** This work invoked two complementary parts. In the first, we performed a theoretical study of various dimers of molecular of titanium dioxide. Five structures were examined. Three among them, the (T), (C) and (T/P) isomers, may be considered as stable compounds because they represent absolute minima on their potential energy surfaces. (T) and (C) may coexist because they are separated by only 6.5 kcal mol<sup>-1</sup> but (T/P) dimer is in a metastable state from an energetic point of view. Non bonded dimer (P) transforms into its homologue (O) which has been considered as transitory specie with low lifetime which evolves to (T) structure. In the second part, we highlight the possible stabilization of (T), (C) and (P) dimers by encapsulation in carbon nanotubes. This indicates the probable role that plays this transitory specie the polymerization process of molecular TiO<sub>2</sub>. Confinement is suitable to control the fast evolution process and could towards the synthesis of new titanium dioxide nanostructured materials. An alternative description of TiO<sub>2</sub> polymorphs (Rutile, anatase et Brookite) is proposed from (T), (C) and (T/P) dimers motifs.

**Keywords :** titanium dioxide, carbon nanotube, confinement, encapsulation, transitory specie

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