

*Electronic Supplementary Information*

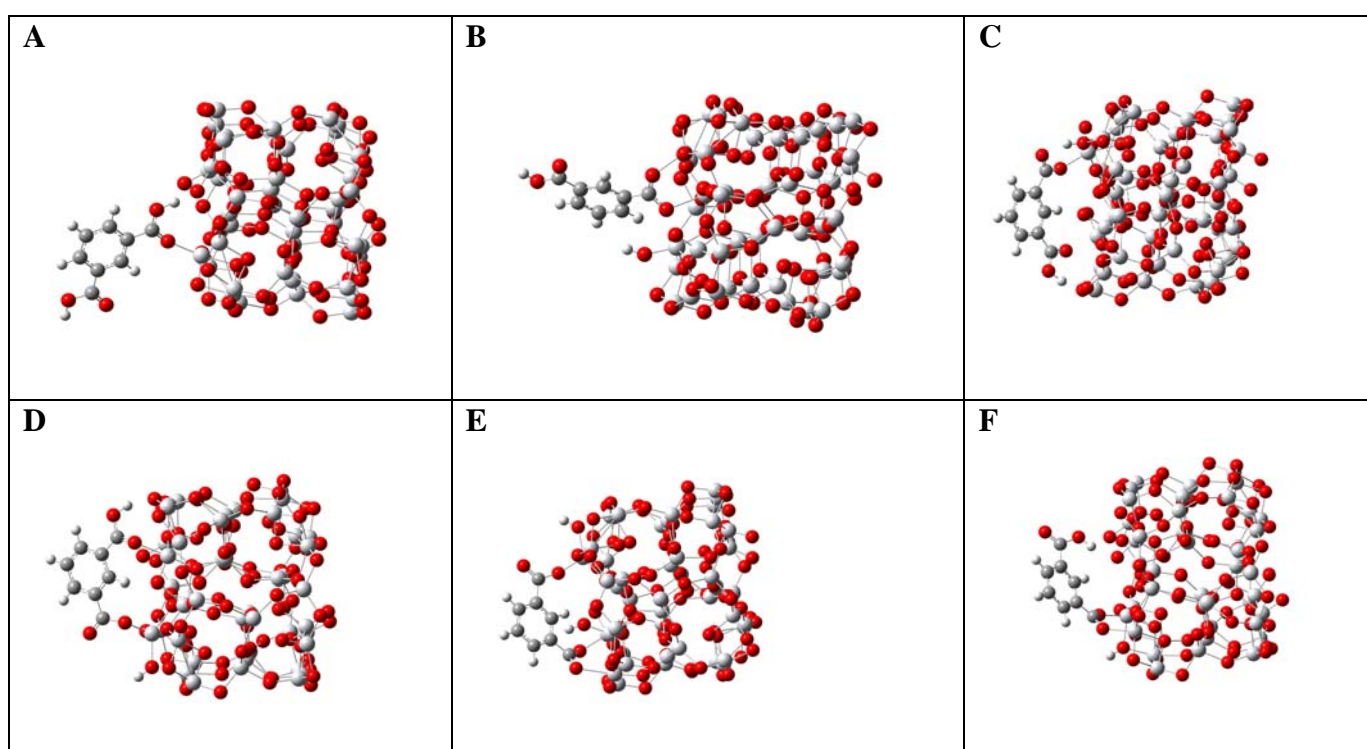
**Calculations of Interfacial Interactions in Pyrene-Ipa Rod Sensitized Nanostructured  
TiO<sub>2</sub>**

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**Figure ESI1.** Fully optimized binding modes A – F of Ipa to (TiO<sub>2</sub>)<sub>46</sub>.