Palmitic acid and hexadecylamine molecules assdsorbed on titania surface in hybrid composites. Effect of surfactants using density functional theory

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A complete theoretical characterization of the factors involved in the stabilization of hybrid laminar composites is reported, with the purpose of understanding the main interactions involved in the formation of these types of systems. The models were built using two different surfactants: hexadecylamine (HDA) and palmitic acid (PAc), on a cluster of titania (TiO2) which represents its anatase crystalline phase. We explored the relevance of the titania-surfactant and surfactant-surfactant interactions, and of the protonation state of the palmitic acid in the stabilization of the hybrid laminar composites. The results were rationalized using energy decomposition analysis (EDA) and the non-covalent interaction index (NIC). The interaction energies between HDA and the TiO2 surface without the contribution of the dispersion forces were ?25 kcal/mol and ?29 kcal/mol for the (1 0 0) and (1 01) surfaces, respectively. These results suggest the formation of a donor-accepto