A first-principle study of the atomic and electronic properties of thymine molecule adsorbed on the Silicon(001) surface

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The chemistry and physics of small organic and biological molecules adsorbed on the Si(001) surface are of fundamental and technological interest, due to the large range of properties that organic molecules can be designed to have and the idea of adding their functionality to semiconductor technology[1]. Moreover, pyrimidinic nucleobases and polycyclic aromatic hydrocarbons (PAHs) have been investigated both experimentally and theoretically[2], due to their role within the framework of origin-of-life models.

In this work we focused on the adsorption of thymine (THY, a pyrimidinic nucleobase) on the Si(001) surface. We calculated atomic and electronic properties of the THY-Si(001) system within a plane-wave (PW) density functional theory (DFT) approach[3], and compared them with those of similar adsorbate systems (tert-butanol[4] and uracil[5]) on the same substrate, in order to investigate the effects of molecule adsorption on the Si(001) surface electronic properties.