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Electronic properties of methyl and hydrogen terminated Si(111) surfaces ANTONIO ALIANO, Physycs Dep., Politecnico di Torino, 10129, Italy, Dept. of Chemistry UC Davis, YAN LI, Dept. of Chemistry UC Davis, GIAN-CARLO CICERO, Dept. of Mat. Science and Chem. Eng., Politecnico di Torino, Italy, GIULIA GALLI, Dept. of Chemistry and Dept. of Physics, UC Davis — Functionalized Si(111) surfaces have many applications in photo-electrochemistry, and some of those (e.g. the use of Si rods as photo-cathodes in solar cell applications) require the development of chemical protection strategies so as to prevent uncontrolled oxidation. Recently [1] a full methylation of Si(111) has been achieved experimentally, which constiutes a promising means to protect Si(111) from oxidation. However, the apparently simple atomic structure of this surface is still under debate. In particular, low temperature STM images appear to yield a pattern in disagreement with structural, first principles optimizations. We have carried out a series of ab-initio calculations of both the structural and electronic properties of the CH3-Si(111) aimed at interpreting STM and STS measurements. A comparison between results obtained at the DFT-GGA level and by using GW calculations will be presented and compared with the corresponding ones for the H-Si(111). This work supported by grant NSF-CHE-0802907 [1]H. Yu et al., Appl. Phys. Lett. 88, 152111, (2006)

Giulia Galli
Dept. of Chemistry and Dept. of Physics, UC Davis

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