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***Ab initio* simulations of alkyl-terminated Si(001) surfaces.** GIANCARLO CICERO, Physics Department, Politecnico of Torino, Torino — Self assembled monolayers (SAMs) are ordered molecular assemblies formed by the adsorption of an active surfactant on a solid surface. The interest in the area of self-assembly, and specifically in SAMs, stems partially from their perceived relevance to science and technology. In contrast to ultrathin films made by, for example, chemical vapour deposition, SAMs are highly ordered and oriented and can incorporate a wide range of groups both in the molecular chain and at the chain termination. Therefore, a variety of surfaces with specific interactions can be produced with fine chemical control. In particular, SAM are used in cantilever based detection, as the first step towards the realization of surfaces with specific sensing properties. Understanding how the surface stress and the mechanical properties of a cantilever change upon functionalization is fundamental to achieve accurate quantitative analysis. Here we present *ab initio* simulations of SAM formation on Si(001) surface to make contact with some recent experimental results [1], in which well packed and ordered alkyl-terminated silicon surfaces were obtained. We will show how the Si(001) surface stress and its mechanical properties (elastic constants) change when organic molecules are attached to it. In particular we will discuss the effect of increasing the surface coverage and the length of the alkyl chain used for the functionalization process. [1] Cerofolini G. F. *Semicond. Sci. Technol.* **18**, 423-429 (2003).

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