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Ab initio study of water molecule dissociation on the hydrogenated Si(100) surface[1] MARILIA J. CALDAS, REGINA LELIS-SOUSA, Institute of Physics, University of Sao Paulo — The reaction mechanisms for the H_2O molecule dissociation at the Si surface, and the resulting oxidation sites, are still object of debate. Here, we present a detailed theoretical investigation of the reaction pathways for the dissociation of water on the Si(100)(2x1):H surface, starting from different initial "attack" sites and leading to different final, oxidized configurations. We use extended-surface (slab) models, working within DFT, with pseudopotentials and plane wave basis set in the quantum-espresso code. The pathways were mapped using the CI-NEB method with both local and gradient corrected exchange-correlation functionals in order to obtain a fair estimate of energy barriers. Our results indicate that the oxidation routes suggested by earlier experimental works are not favored. We propose two new oxidation routes, with simultaneous release of one H2 molecule: one related to chemisorption of the oxygen atom on the Si-Si dimer bond, and another related to the absorption on the back-bond. Analysis of energy barriers showed that these two new possibilities are both kinetically and energetically viable. We also present analyses of the profiles obtainable through STM for the investigated structures, which should help experimental identification.

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