

Abstract Submitted  
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***Ab initio* molecular dynamics of a proton in amorphous SiO<sub>2</sub> illustrating the hopping mechanism** JULIEN GODET, ALFREDO PASQUARELLO, Ecole Polytechnique Fédérale de Lausanne, Institute of Theoretical Physics, CH-1015 Lausanne — The scaling of metal-oxide-semiconductor devices to smaller dimensions is a major issue in current silicon technology. In order to understand the role of hydrogen at silicon-oxide interfaces, we here investigate charged states of hydrogen in amorphous SiO<sub>2</sub> (*a*-SiO<sub>2</sub>) using first-principles calculations (DFT-GGA). We first show that the formation energies of H<sup>0</sup>, H<sup>+</sup> and H<sup>-</sup> in *a*-SiO<sub>2</sub> are essentially equivalent to those in  $\alpha$ -quartz. In particular, the H<sup>+</sup> and H<sup>-</sup> species are always more stable than their neutral counterpart. Then, we focus on the basic diffusion mechanism of the proton in *a*-SiO<sub>2</sub>. Our molecular dynamics simulations show that the proton hops between O atoms. The hopping does not occur between first O neighbors connected through the network, but takes place across rings when the O–O distance is about 2.3 Å. The hopping process is favored by the thermal vibrations of the O atoms.

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