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Formation and reactions of hydronium species in silica I.G. BATYREV, L. TSETSERIS, S.T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235 — Water-related impurities in silica-based glasses are known to affect the properties of the network and corresponding devices in many types of ways. Here, we use first-principles calculations to highlight the special role of one of these species, hydronium (H_3O). We elucidate the atomic-scale details of formation and reactions of H_3O molecules in amorphous SiO_2. We find that the attachment of a migrating H^+ on a water molecule is an exothermic reaction with an energy gain of 0.4 eV and activation energy of only 0.6 eV. We present results on pertinent features in the vibrational spectra of silica that support the presence of H_3O, and we describe the role of H_3O as a passivant of oxide defects, like oxygen vacancies and non-bridging oxygen atoms, and the atomic-scale details of H_3O-mediated diffusion of H species in SiO_2. The results bear on the formation and dynamics of defects in electronic devices and the physical properties of hygroscopic silica-based glasses. This work was supported in part by the AFOSR and the US Navy.

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