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Role of the three Si suboxides at the surface of Si quantum dots and in Si/SiO_2 quantum wells on optical response[1] PIERRE CARRIER, University of Minnesota — The Si/SiO_2 interface structure has been extensively studied in the past, especially for MOSFET applications. Recent applications of Si/SiO_2 nanostructures in solar cells and LEDs are now investigated using Si quantum dots (QD) or Si/SiO_2 quantum wells (QW). The Si/SiO_2 interface contains three Si suboxides, each bonded to 1, 2, or 3 oxygen atoms, respectively referred to as Si^{1+}, Si^{2+}, and Si^{3+}. Models that contain all three suboxides are difficult to construct; results in the literature on oxygenated Si QD usually include Si^{1+} and Si^{2+} only. The models presented here contain the 3 suboxides and are based on a Si/SiO_2 surface model originally constructed by Pasquarello *et al.*, Appl. Phys. Lett. **68**, 625 (1996). This model was used later by the author in the study of Si/SiO_2 QW [Phys. Rev. B **65**, 165339 (2002)] and is now extended to Si QD. It is shown that the band gap or optical response depends strongly on the Si suboxide atomic configuration at the surface of QD or at the interface of QW. Trends on the band gap variations as function of the three suboxides will be discussed. All models (QW and QD) are structurally relaxed using the program PARSEC [Phys. Rev. Lett. **72**, 1240 (1994)].

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