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Interface chemistry of silicon nanocrystals embedded in silica[1]
DUNDAR YILMAZ, CEYHUN BULUTAY, Bilkent University, TAHIR CAGIN, Texas A&M University — Molecular dynamics simulations of realistic-sized silicon nanocrystals (NCs) with the diameters in the range from 1 nm to 3 nm embedded in amorphous oxide are carried out till steady state conditions with the chemical environment described by the reactive force field model. We identify different types of three-coordinated oxygen (3cO) complexes, previously not noted, on the oxide interface. No double bonds were observed. We reveal that the interface bond topology evolves among different oxygen bridges through these 3cO complexes. The abundance and the charge distribution of each oxygen complex is determined as a function of the NC size as well as the transitions among them. The number of bridge bonds is observed to scale with surface area, thus the curvature has a small effect on the number of bridges. Among the three bonds of 3cO, the weaker bond is more susceptible to bond breaking which is also likely to take part in an optical activity through bond breaking and reformation. Our results indicate that the Si NC-oxide interface is more complicated than the previously proposed schemes which were based on solely double and bridge bonds.

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