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Electronic Properties of Defects at the Surface of Embedded Silicon Nanoparticles NICHOLAS BRAWAND, MARTON VOROS, Univ of California - Davis, GIULIA GALLI, IME, The University of Chicago — Using density functional theory calculations we predicted the single particle energies and lifetimes of dangling bond defects at the surface of various Si nanoparticles (NPs) embedded in amorphous SiO_2 matrices [1]. We found that both the lifetimes and the single particle excitation energies of these defects depend on the size of the NP. However, the energy positions of the dangling bond defect levels are always within the NP gap, irrespective of size, between 1 and 2 nm. Our findings suggest that the presence of silicon NPs within amorphous SiO_2 may impact the functionality of silicon-on-insulator nanophotonic devices operating near 1.5 μm [2]. [1] Li, Tianshu et al. Phys. Rev. Lett., 107, 206805 (2011) [2] Bogaerts, W. et al. Journal of Lightwave Technology, 23, 401-412 (2005)

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