

Abstract Submitted
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Electronic origin of photoluminescence from Si nanocrystal embedded in amorphous SiO₂ matrix¹ TIANSHU LI, Department of Civil and Environmental Engineering, George Washington University, FRANCOIS GYGI, Department of Applied Science & Department of Computer Science, University of California, Davis, GIULIA GALLI, Department of Chemistry & Department of Physics, University of California, Davis — Through combining classical molecular dynamics and *ab initio* calculation, we have created composite models of Si nano crystal embedded in SiO₂ amorphous matrices, with the sizes of Si nanocrystals ranging from 1.3 nm ~ 1.9 nm. Electronic structure calculations showed that the band gap of composite structure increases as the size of Si nanocrystal reduces, however the increase of gap is mainly attributed to the *lowering of valence band edge*, with conduction band edge virtually unchanged. It was also found that while the wavefunctions from conduction band edges are extended over the entire Si nanocrystal, those from the valence band edges are mainly distributed near the nanocrystal/matrix interface. Further analysis identified that the valence band edges are dominated by the local distortion of nanocrystal from diamond cubic structure, which increases as both approaching the surface of Si nanocrystal, and decreasing the size of Si nanocrystal. This finding suggests that the local strain induced by surrounding amorphous SiO₂ matrix may play a key role in the photoluminescence of Si nanocrystal/SiO₂ amorphous matrix composite structures.

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