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Surface Dangling Bonds Are a Cause of Type-II Blinking in Si Nanoparticles[1] NICHOLAS BRAWAND, MARTON VOROS, GIULIA GALLI, Univ of Chicago — Exponential blinking statistics was reported in oxidized Si nanoparticles and the switching mechanism was attributed to the activation and deactivation of unidentified nonradiative recombination centers. Using ab initio calculations we predicted that Si dangling bonds at the surface of oxidized nanoparticles introduce defect states which, depending on their charge and local stress conditions, may give rise to ON and OFF states responsible for exponential blinking statistics. Our results are based on first principles calculations of charge transition levels, single particle energies, and radiative and nonradiative lifetimes of dangling bond defects at the surface of oxidized silicon nanoparticles under stress.

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