Title: Conical intersections in silicon clusters with dangling bond defects: the effects of cluster size Authors: Wei-Tao Peng, B. Scott Fales, and Benjamin G. Levine

Silicon dangling bond defects are known to act as non-radiative centers. We have previously shown that there are low-lying conical intersections capable of facilitating non-radiative recombination in a small silicon cluster (Si8H10) with a dangling bond defect. However, the situation in realistic nanometer-sized clusters had yet to be examined. On the other hand, since nanoparticles of various sizes can be synthesized, it is desirable to know how the size of the silicon cluster affects non-radiative processes. In this study, we investigate particle-size effects on the location and energy of conical intersections. With the aid of a graphical processing unit (GPU) accelerated implementation of the complete active space configuration interaction (CASCI) method, the calculations for searching conical intersections in nanoparticles are now feasible. Such intersections are identified in clusters up to  $\sim 1.3$  nm in diameter.