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Vacancy-related defects and the E'$_\delta$ center in amorphous silicon dioxide BLAIR TUTTLE, Penn State Erie, SOKRATES PANTELIDES, Vanderbilt University — The microscopic identification of vacancy-related defects in silicon dioxide has been a major challenge. Particularly in amorphous silica, the role of vacancy clusters is still controversial. Experimental data have led to suggestions that the E'$_\delta$ center is a four-vacancy cluster instead of a single vacancy. Here we report density functional calculations of single vacancies and clusters of four vacancies in realistic models of amorphous silica. Results for single vacancies compare well to previous theory. A key result for four-vacancy clusters is that relaxations localize the unpaired electron preferentially on one Si atom, resulting in a strongly anisotropic electron-paramagnetic-resonance signal. Electrons at single vacancies have a more benign anisotropy which is more compatible with the observed isotropic signal. This work was supported by the Air Force Office of Scientific Research under a MURI grant (FA9550-05-1-0306) and by the US Navy.

Blair Tuttle
Penn State Erie

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