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**First-Principles Investigation of Low Energy E' Center Precursors in Amorphous Silica** NATHAN ANDERSON, School of Materials Engineering, Purdue University, RAVI VEDULA, School of Electrical and Computer Engineering, Purdue University, PETER SCHULTZ, Sandia National Laboratories, RENEE VAN GINHOVEN, Pacific Northwest National Laboratory, ALEJANDRO STRACHAN, School of Materials Engineering, Purdue University — We show that oxygen vacancies are not necessary for the formation of E' centers in amorphous SiO2 and that a single O-deficiency can lead to two charge traps. Employing molecular dynamics with a reactive potential and density functional theory we generate an ensemble of stoichiometric and oxygen-deficient amorphous SiO2 atomic structures and identify low-energy network defects. Three-coordinated Si atoms appear in several low-energy defects both in stoichiometric and O-deficient samples where, in addition to the neutral oxygen vacancy, they appear as isolated defects. Various charge transition levels for each defect are also presented.

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