Abstract Submitted
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First principles calculations of the Urbach tail in the optical absorption of silica glass[1] BABAK SADIGH, Lawrence Livermore National Laboratory, PAUL ERHART, Chalmers University of Technology, DANIEL ABERG, ERIC SCHWEGLER, JEFF BUDE, Lawrence Livermore National Laboratory, OPTIC DAMAGE MODELING TEAM — We present density-functional theory calculations of the optical absorption spectra of silica glass for temperatures up to 2400 K. The calculated spectra exhibit exponential tails near the fundamental absorption edge that follow the Urbach rule, in good agreement with experiments. We also discuss the accuracy of our results by comparing to hybrid e xchange correlation functionals. By deriving a simple relationship between the exponential tails of the absorption co efficient and the electronic density-of-states, we establish a direct link between the photoemission and the absorpti on spectra near the absorption edge. This relationship is subsequently employed to determine the lower bound to the U rbach frequency regime. Most interestingly, in this frequency interval, the optical absorption is Poisson distributed with very large statistical fluctuations. Finally, We determine the upper bound to the Urbach frequency regime by id entifying the frequency at which transition to Poisson distribution takes place.

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