

Abstract Submitted
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Temperature- and pressure-induced changes in optical properties of silica ANDREA TRAVE, BABAK SADIGH, ERIC SCHWEGLER, JEFF BUDE, Lawrence Livermore National Laboratory — Silica is among the most commonly studied materials in its crystalline and amorphous forms, yet it still presents several obscure aspects in its behavior under heating and densification. First-principles simulations of silica glass and quartz are conducted to explain the experimentally observed rapid increase in optical absorption and consequent defect formation when silica glass is heated. Prior to full gap closure, we observe the appearance of optically active localized states, which will be studied in terms of their origin and characterization. Additional analysis of the effect of localized structural defects and of the optical properties of the material under compression will also be undertaken and discussed. This work was performed under the auspices of the US Department of Energy by the University of California at the LLNL under contract no W-7405-Eng-48.

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