

Abstract Submitted
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Core level XAS study on high pressure solids MIN WU, JIANZHONG JIANG, Zhejiang University, JOHN TSE¹, University of Saskatchewan — We investigated the K and L-edge core level X-ray absorption spectra of solid CO₂ and Silica (SiO₂) under high pressure, using methods based on pseudopotentials and all-electron Bethe-Salpeter Equation. A comparison of the calculated spectra with both methods is present. We found that the calculated Si K and L-edge spectra of quartz and stishovite are in good agreement with experiment. Particularly, the origin of the second peak in the O K-XAS observed in compressed silica which is often used as an indication of six-fold coordinate is explained. Preliminary calculations show both the full core hole and no core hole approximations failed to reproduce quantitatively the observed C and O K-edge XAS.

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