

Abstract Submitted
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Crystal Structure and Lattice Dynamics of Fe-Si Alloys under High Pressure YI ZHANG, RAVHI KUMAR, Department of Physics and Astronomy and HiPSEC, University of Nevada, Las Vegas, ZACKARI FISK, Department of Physics and Astronomy, University of California, Irvine, YUMING XIAO, MICHAEL HU, PAUL CHOW, HPCAT and Carnegie Institution of Washington, Advanced Photon Source, Argonne National Laboratory, Argonne, ANDREW CORNELIUS, CHANGFENG CHEN, Department of Physics and Astronomy and HiPSEC, University of Nevada, Las Vegas — The crystal structure and lattice dynamics of Fe-Si alloys under high pressures up to 115 GPa are studied by first-principles density functional theory (DFT) calculations. Our results agree well with the X-ray diffraction and nuclear inelastic x-ray scattering experiment. The calculated thermodynamic properties and sound velocities give new insights to the studies of Earth's core.

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