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Physics of matter at extreme conditions: insights from quantum mechanical calculations¹

SHUAI ZHANG, Lawrence Livermore Natl Lab

Knowledge about structures and properties of matter at high pressure, temperature conditions are extremely important for understanding planetary interiors, simulating post-giant impact processes, and the design and interpretation of high-energy-density (HED) experiments. By means of quantum mechanical calculations, we study chemical bond dissociation, phase transformation, and equations of state in representative materials or rock-forming minerals under dynamic compression. We characterize the physical processes from the atomistic and electronic levels, compare our findings with experiments and previous calculations, quantify fidelity of the results, and discuss implications for planetary and HED sciences. This is an effort toward unambiguous elucidation of extreme physics.

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