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Theoretical Mineral Physics for Study on Earth's Deep Interior

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Recent progress in theoretical and computational mineral physics based on the density functional techniques has been dramatic in conjunction with the advancement of computer technologies. It is now possible to predict phase stability and several physical properties of complex minerals quantitatively in the pressure and temperature conditions corresponding directly to the deep planetary interiors with uncertainties that are comparable to or even smaller than those attached in experimental data. Our challenges include calculations of phase equilibria of planetary materials up to terapascal pressures (1-3), high-pressure and high-temperature elasticity to constrain the thermochemical property of the Earth (4,5), and thermal, electrical, and mass transport properties to investigate the planetary dynamics (6-8).

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