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Pure Iron Compressed and Heated to Extreme Conditions

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The results of a first-principles study supported by the temperature-quenched laser-heated diamond anvil-cell experiments on the high-pressure high-temperature structural behavior of pure iron are reported. We show that in contrast to the widely accepted picture, the face-centered cubic (fcc) phase becomes as stable as the hexagonal close-packed (hcp) phase at pressures around 300-360 GPa and temperatures around 5000-6000 K. Our temperature-quenched experiments indicate that the fcc phase of iron can exist in the pressure-temperature region above 160 GPa and 3700 K, respectively. This, in particular, means that the actual structure of the Earth's core may be a complex phase with a large number of stacking faults.