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**The pressure-induced bcc-hcp structural transformation in iron**

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We study within the framework of the spin density-functional theory the microscopic mechanism of the bcc-to-hcp martensitic transformation in iron from first principles. We investigate the correlation of the pressure-induced structural instability of the bcc phase with the disappearance of ferromagnetism in this system. We show that our calculations can shed new light on recent novel shock experiments in single-crystalline iron.

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