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Quantum Monte Carlo calculates bulk properties and magnetic ordering in iron[1] WILLIAM D. PARKER, JOHN W. WILKINS, Ohio State University — Quantum Monte Carlo (QMC) models electronic systems with high accuracy but its computational demands limit wider use. Few QMC calculations exist for solid-state systems and none comparing the energetic ordering of different spin configurations (magnetic states). Density-functional calculations with generalized-gradient-approximation exchange-correlation give correct magnetic ordering and accurate lattice constants and bulk moduli for bcc iron. However, the predicted cohesive energy differs from experiment by 0.5-1.0 eV. QMC-calculated bulk elastic properties for pure iron in the bcc, hcp and fcc phases compare with properties in the ferromagnetic, antiferromagnetic and nonmagnetic spin configurations.

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