

Abstract Submitted
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Ortho-para transition of interstitial H₂ in Si¹ MICHAEL STAVOLA, CHAO PENG, MEGAN LOCKWOOD, Lehigh University — Interstitial H₂ in Si is a nearly-free rotator and has ortho and para species with the nuclear spins of the two protons aligned either parallel or antiparallel [1]. If one waits a sufficiently long time at low temperature, H₂ will relax to its lower energy para state. The ortho-para (o-p) transition for H₂ in Si has been observed in recent Raman studies [2]. We have performed IR absorption experiments to investigate issues that have proved difficult to study by Raman. When a Si sample containing H₂ is stored for a month or more at 77K, the 3618.4 cm⁻¹ IR line assigned to o-H₂ [1] is reduced in intensity because, when the o-p transition occurs, p-H₂ is not seen by IR. When this sample was annealed at room temperature, the ortho population characteristic of room temperature was recovered with a time constant of ≈6 hrs. Our IR studies of the kinetics of the o-p transition complement recent Raman results and suggest that the cause of the o-p transition is not yet understood.

[1] M. Stavola *et al.*, Physica B **340-342**, 58 (2003).

[2] M. Hiller *et al.*, Phys. Rev. Lett. **98**, 055504 (2007); **99**, 209901 (2007).

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