Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Reentrant Phase Diagram in Ortho-Para Mixtures of Solid H_2 at High Pressure BALAZS HETENYI[1], SISSA, Trieste (Italy), SANDRO SCANDOLO, The Abdus Salam ICTP and INFM-CNR Democritos, Trieste (Italy), ERIO TOSATTI, SISSA, ICTP, and Democritos, Trieste (Italy) — Quantum effects dominate the low temperature phase diagram of solid molecular hydrogen in a wide range of pressures from ambient up to about 100 GPa. Important differences exist in the behavior of pure even-J(para-H_2 and ortho-D_2), and odd-J (ortho-H_2 and para-D_2) species, but little is known about the phase diagram of ortho-para mixtures. We develop a multiorder parameter mean-field formalism for systems of coupled quantum rotors and apply it to solid H_2 and D_2. For a thermal distribution of ortho-para molecules we find an anomalous reentrant orientational phase transition in the pressure - temperature phase diagram of both systems [Hetenyi et al., PRL 94, 125503 (2005)]. The correlation functions of the order parameter indicate short-range order at low temperatures. As the temperature is increased the correlation increases along the phase boundary. We also find that even extremely small *odd-J*concentrations (1%) can trigger short-range orientational ordering.

[1]present address: TU Graz, Austria

Sandro Scandolo
The Abdus Salam ICTP

Date submitted: 30 Nov 2005 Electronic form version 1.4