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Y. Crespo*, A. Laio, G. E. Santoro, M. Fabrizio,
S. Scandolo, E. Tosatti

International Center for Theoretical Physics, StradaCostiera, Trieste, Italy
*E-mail: ycrespo@ictp.it

Unconventional phase transitions on HD and O_2 cryocrystals

Both HD and O_2 are molecular solids with an exceedingly well explored phase diagram under pressure. In this talk we focus in two unusual phase transition taking place at high pressures. First we study the unusual reentrant phase transition that the phase diagram of HD exhibits near 50 Gpa where a rotationally ordered ("broken symmetry") crystalline phase surprisingly transforms into a rotationally "disordered" high-symmetry phase upon cooling.

Key words: phase diagram, pressure, sample, crystalline phase.

Ю. Креспо, А. Лайо, Г.Е. Санторо, М. Фабрицио, С. Скандоло, Е. Тосатти

Нетрадиционные фазовые переходы в HD и O_2 криокристаллах

Обе молекулы HD и O_2 твердых тел обусловлены хорошо изученной фазовой диаграммой при высоких давлениях. В этом докладе мы фокусируем внимание на двух необычных фазовых переходах, существующих при высоких давлениях. Первоначально мы изучим необычный, возвратный фазовый переход, на фазовой диаграмме HD образцов в окрестности 50 ГПа, где вращение обнаруживает «нарушение симметрии» кристаллической фазы, обусловленное превращением в «неупорядоченной» стадии высокой симметрии при охлаждении.

Ключевые слова: фазовая диаграмма, давление, образцы, кристаллическая фаза.

Ю. Креспо, А. Лайо, Г.Е. Санторо, М. Фабрицио, С. Скандоло, Е. Тосатти

Криокристалдардағы HD және O_2 дәстүрлі емес фазалық ауысулар

HD және O_2 қатты денелердің қос молекулалары жоғары қысымдағы жақсы зерттелген фазалық диаграммаға негізделген. Бұл баяндамада біз жоғары қысымда болатын екі ерекше фазалық ауысуларға назар аударамыз. Алдымен біз, HD үлгінің фазалық диаграммасындағы айналу («симметрияның бұзылуы») ауысуын зерттедік.

Түйін сөздер: фазалық диаграмма, қысым, үлгілер, кристалдық фаза.

Both HD and O_2 are molecular solids with an exceedingly well explored phase diagram under pressure. In this talk we focus in two unusual phase transition taking place at high pressures. First we study the unusual reentrant phase transition that the phase diagram of HD exhibits near 50 Gpa where a rotationally ordered («broken symmetry») crystalline phase surprisingly transforms into a rotationally «disordered» high-symmetry phase upon cooling. While the qualitative reason for reentrance, has been already shown by early mean field studies in this work.We aiming at a quantitative understanding of this system using path integral Monte Carlo (MC) constant-pressure calculations. Here we use an efficient sampling method and found the lowest-energy zero-temperature classical state, an structure C_2/c similar to that hypothesized by Surh et al. [Phys. Rev. B 55, 11330 (1997)]. Upon turning quantum rotational effects on, we calculate the pressure-temperature phase diagram by monitoring a lattice biased order parameter, and find a reentrant phase boundary in good agreement with experiment. The entropy jump across the transition is found to be comparable with ln 2, the value expected from mean field results. A comparison with earlier studies is also presented, yielding relevant information about the role of factors that quantitatively determine the reentrant part of the phase diagram. The second part of the talk is devoted to molecular oxygen at high pressures. At low temperatures, the low pressures antiferromagnetic phases below 8 GPa where O_2 molecules have spin *S*=1 are followed by the broad apparently nomagnetic epsilon phase from about 8 to 96 GPa. In this phase which is our focus molecules group structurally together to form quartets while switching, as believed by most, to spin *S*=0. In this work we present theoretical results strongly connecting with existing vibrational and optical evidence, showing that this is true only above 20 GPa, whereas the *S*=1 molecular state survives up to at about 20 GPa. The epsilon phase thus breaks up into two: a spinless epsilon_0 (20-96 GPa), and another epsilon_1 (8-20 GPa) where the molecules have *S*=1 but possess only short range antiferromagnetic correlations. Thus an unconventional and rare local spin liquid-like singlet ground state akin to some earlier proposals and whose optical signature we identify in existing data, is proposed for this phase. Our proposed phase diagram thus has a first order phase transition just above 20 GPa, extending at finite temperature and most likely terminating into a crossover with a critical point near 30 GPa and 200 K.