

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Hydrogen bond symmetrization by proton quantum motion and high Tc superconductivity in Sulfur hydrides at high pressure.** ION ERREA, University of the Basque Country and Donostia International Physics Center, MATTEO CALANDRA, CNRS and Université P. et M. Curie, CHRIS PICKARD, University College London, JOSEPH NELSON, RICHARD NEEDS, Cavendish Laboratory Cambridge, Y LI, HANYU LIU, University of Saskatchewan, YUNWEY ZHANG, YAMMING MA, State Key Laboratory of Superhard Materials,, FRANCESCO MAURI, CNRS and Université P. et M. Curie — Atoms in a crystal are quantum particles differing substantially from classical particles. The vibrational energy associated to the quantum oscillations can strongly modify the static energy landscape, even changing the ground state derived from the Born-Oppenheimer energy surface (BOES) minimum. Here, making use of density-functional theory and of the Stochastic Self-consistent Harmonic Approximation, we show that the ground state of the high Tc superconductor hydrogen sulfide at 155 GPa is completely determined by quantum fluctuations. Indeed, despite the minimum of the BOES is obtained for a rhombohedral structure with covalently bonded H3S units and hydrogen bonds between them, quantum fluctuations favor a fully symmetric cubic structure in which the covalent and hydrogen bonds equalize. The quantum hydrogen-bond symmetrization and the large anharmonic effects are crucial to understand the pressure dependence of the observed extraordinary  $T_c=205$  K at 155 GPa. We finally show how, the dependence of  $T_c$  as a function of pressure can be completely explained in the framework of a phonon mediated pairing mechanism in the presence of large anharmonic effects.

Matteo Calandra  
CNRS and Université P. et M. Curie

Date submitted: 01 Nov 2015

Electronic form version 1.4