

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Pressure-induced Superconductivity in the Hydrogen-dense material YH_3 ¹ DUCK YOUNG KIM, TCM group, Cavendish laboratory, 19 J J Thomson Avenue, Cambridge CB3 0HE, UK, RALPH SCHEICHER, RAJEEV AHUJA, CMT group, Uppsala University, Sweden — The results presented by us allow for an understanding of pressure-induced superconductivity of tri-hydrides with a particular focus on YH_3 . We show that a structural phase transition from hexagonal to cubic structure occurs at 20 GPa, which is in good agreement with recent experiments. This structural phase transition is seen to be accompanied by an insulator-to-metal transition in our quasi-particle calculations. Furthermore, we present an analysis of the superconducting behavior in cubic YH_3 . At the lowest possible pressure (17.7 GPa), cubic YH_3 is superconducting with a T_c of 40 K and turns into the normal metallic phase at 25 GPa due to a change of s-d hybridization between hydrogen and yttrium. This hitherto unprecedented low pressure should make superconducting YH_3 a very attractive system to study experimentally among the hydrogen-rich superconductors. Finally, we also predict that the superconducting phase reemerges at 45 GPa. J. S. de Almeida, D. Y. Kim, C. Ortiz, M. Klintenberg, and R. Ahuja, *Appl. Phys. Lett.* **94** 251913 (2009). D. Y. Kim, R. H. Scheicher, R. Ahuja, *Phys. Rev. Lett.* **103**, 077002 (2009).

¹Wenner-Gren foundation in Sweden, The Royal Society in UK

Duck Young Kim
TCM group, Cavendish laboratory,
19 J J Thomson Avenue, Cambridge CB3 0HE, UK

Date submitted: 18 Nov 2009

Electronic form version 1.4