ID de Contribution: **10** Type: **Poster**

Energy Gap Closure of Crystalline Molecular Hydrogen with Pressure

mardi 16 mars 2021 15:32 (2 minutes)

We study the gap closure with pressure in Phases III and IV of molecular crystalline hydrogen by Quantum Monte Carlo methods [1]. Nuclear quantum and thermal effects are considered from first principles with Coupled Electron Ion Monte Carlo. The fundamental electronic gaps are obtained from grand-canonical Quantum Monte Carlo methods [2] properly extended to quantum crystals. Nuclear zero point effects cause a large reduction in the gap (~2eV). As a consequence the fundamental gap closes at 530GPa for ideal crystals while at 360GPa for quantum crystals. Since the direct gap remains open until ~450GPa, the emerging scenario is that upon increasing pressure in phase III (C2/c-24 crystal symmetry) the fundamental (indirect) gap closes and the system enters into a bad metal phase where the density of states at the Fermi level increases with pressure up to ~450GPa when the direct gap closes. Our work partially supports the interpretation of recent experiments in high pressure hydrogen.
[1] Phys. Rev. Letts.1 24, 116401 (2020)
[2] Phys. Rev. B 101, 085115 (2020)

Language

English

Field

Auteurs principaux: GORELOV, Vitaly (Ecole Polytechnique); CEPERLEY, David M. (University of Illinois at Urbana-Champaign); HOLZMANN, Markus (Univ. Grenoble Alpes, CNRS); PIERLEONI, Carlo (University of L'Aquila)

Orateur: GORELOV, Vitaly (Ecole Polytechnique)

Classification de Session: Poster advertising session

Classification de thématique: Physics