

Dense Hydrogen Can Behave Like Topological Insulator

10/2016

Scientific Achievement

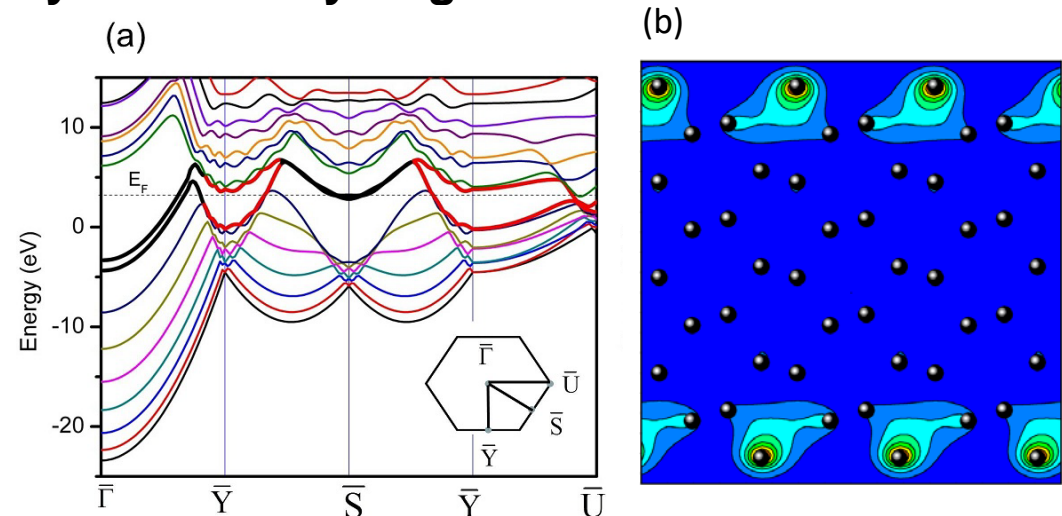
It was shown that dense hydrogen can have metallic surface states even when the bulk of material remains insulating.

Significance and Impact

The results provide predictions for future measurements, including probes of possible surface superconductivity in dense hydrogen.

Research Details

- First-principles calculations of band structures, Zak's phases and charge densities of dense phases of hydrogen.
- Two-dimensional distributions of Zak's phase were used to predict the existence of topological surface states on some particular surfaces.
- Surface states were calculated within a supercell approach, *i.e.* for thin films periodically repeated along the normal direction at equal vacuum gaps.



Topological surface states in a 4-unit cell thick $Cmca-4$ structure. (a) Surface band structure. The surface states are indicated by thick black curves. (b) The charge density of the lower surface state at the \hat{S} point.

Naumov I. I. and Hemley R. J. Topological Surface States in Dense Solid Hydrogen, *Phys. Rev. Lett.* **117**, (2016), in press.