

Abstract Submitted
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First-principles study of polar molecule adsorption on hydrogenated diamond (001)¹ YONG-HYUN KIM, S. B. ZHANG, National Renewable Energy Laboratory, YANG YU, L. F. XU, C. Z. GU, Chinese Academy of Sciences — Density functional theory calculations reveal that adsorption of small polar molecules such as H₂O, HF, and HCl on hydrogenated diamond (001) surfaces can result in unexpected dihydrogen bonding. This implies that in a C-H bond, H may be more electronegative than C, thus deviating from the widely-accepted Pauling's electronegativity scale, C(2.55) *vs* H (2.20). Detailed analysis of the self-consistent charge densities confirms that electrons are indeed accumulated more at the H site than at the C site with respect to the free atoms. It further explains why dihydrogen bond can form for H₂O and HF on the surfaces, but not for NH₃. The true physical origin for the well-known reduction of the work function due to surface hydrogenation is now attributed to the replacement of loosely bonded surface C π electrons by more tightly bonded C-H σ electrons. We also propose that the favorable formation of the dihydrogen bonds may contribute to the observed p-type conductivity of diamond surfaces in acidic conditions.

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