Metastable Structures and Recombination Pathways for Atomic Hydrogen on the Graphite(0001) Surface

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Abstract. Combined Scanning Tunnelling Microscopy (STM) and Density Functional Theory (DFT) investigations show that hydrogen atoms cluster on the graphite (0001) surface due to preferential sticking into specific adsorbate structures. After annealing to temperatures sufficiently high for atomic recombination and molecular desorption to set in, two well defined dimer states appear on the surface. Density functional theory calculations reveal that the stability of these structures is not determined by their binding energy but by their kinetic stability towards atomic recombination. Direct recombination is only possible from one of the dimer states. This results in increased stability of one dimer species and explains the puzzling double peak structure observed in temperature programmed desorption spectra for hydrogen on graphite.