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Interaction of H atom with Si(111)4x1-In surface SANG-YONG YU, Korea Research Inst. of Standards and Science, GEUNSEOP LEE, Inha Univ., Inchon, Korea, HANCHUL KIM, Korea Research Inst. of Standards and Science, D. LEE, Chungnam Univ., Daejeon, Korea, JA-YONG KOO, Korea Research Inst. of Standards and Science — Using scanning tunneling microscopy (STM) measurements and *ab initio* calculations, the interaction of an H atom with the Si(111)4x1-In surface at room temperature is investigated. It is found that the H atom preferentially adsorbs at the bridge site between the In chain and the Si Seiwatz chain and break an In-Si bond to form a Si-H bond. Experimentally, the adsorption of H is influenced by the registry of the Si substrate and preferentially occupies one of the two zigzag In chains to the other, while the little difference is found in the calculated adsorption energy. The adsorbed H atom induces not only a localized lattice distortion but also a distant electronic perturbation near the Fermi level, which appears as out-of-phase period-doubled (x2) charge ordering in the filled- and the empty-state STM images. These perturbations induced by the two nearby H atoms in the same row interfere to make the inbetween x2 modulation enhanced or suppressed depending on the H-H distance. The x2 perturbed region remains metallic, distinguishing it from the insulating low-temperature 4x2 (8x2) phase. The observed x2 perturbation away from the H-adsorbate is found to be the theoretical ground state of the In/Si(111) surface predicted by density-functional theory, which is stabilized by the presence of the surface defect.

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