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Phosphine Adsorption and Dissociation on the Si(001) Surface: An Ab Initio Survey of Structures OLIVER WARSCHKOW, HUGH F. WILSON, NIGEL A. MARKS, DAVID R. MCKENZIE, Centre for Quantum Computer Technology, School of Physics, University of Sydney, Australia , STEVEN R. SCHOFIELD, NEIL J. CURSON, MICHELLE Y. SIMMONS, Centre for Quantum Computer Technology, School of Physics, University of New South Wales, Australia, PHIL V. SMITH, MARIAN W. RADNY, School of Mathematical and Physical Sciences, University of Newcastle, Callaghan, Australia — The continued downscaling of electronic components to the atomic scale leads to a number of novel devices including quantum cellular automata, single electon transistors and quantum computers. The fabrication of such devices invariably requires scanning probe microscopies and an atomic-level understanding of doping mechanisms and the intermediate species involved. In the case of phosphorus, it is well established that PH_3 adsorbs dissociatively on the Si(001) surface, much controversy surrounds the numerous intermediate species observed in STM experiments. We present an extensive density functional theory (DFT) survey of possible PH_3 dissociation products and assign three prominent STM features as PH_2, PH and P species, respectively. All three structures are fully consistent with STM data and collectively outline a mechanism for the complete PH_3 dissociation on the Si(001) surface.

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