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Mechanism of Phosphine Dissociation on the Si(001) Surface 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 down-scaling of electronic devices to the atomic scale increasingly requires an atomic-level understanding of the elementary processes of semiconductor doping. We present a combined experimental and theoretical investigation into the dissociation mechanism of phosphine (PH3) on the Si(001) surface. As reported by us elsewhere in this conference, a number of prominent intermediate species of PH3 dissociation observed in STM experiments have been structurally characterized as PH2+H, PH+2H and P+3H species respectively. In this poster we present detailed quantum chemical calculations of these and other short-lived intermediates as well as the transition (kinetic) barriers between them. This leads us to formulate a step-by-step mechanism for the complete dissociation of PH3 on the Si(001) surface.

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