

Abstract Submitted
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The reaction of arsine (AsH_3) with the silicon (001) surface. Similar to phosphine (PH_3), or completely different? OLIVER WARSCHKOW, The University of Sydney, STEVEN SCHOFIELD, London Centre for Nanotechnology, NIGEL MARKS, Curtin University, DAVID MCKENZIE, The University of Sydney, NEIL CURSON, London Centre for Nanotechnology — The $\text{AsH}_3/\text{Si}(001)$ chemisorption system is of potential utility to the fabrication of atomic-scale Si:As devices using scanning tunneling microscopy hydrogen lithography techniques. This follows from the notion that AsH_3 is chemically analogous to phosphine (PH_3) for which the corresponding Si:P lithography techniques are becoming well established (see e.g. Ref. 1). This talk uses density functional theory to explore the initial adsorption reaction of an AsH_3 molecule, and its stepwise breakdown into AsH_2+H , $\text{AsH}+2\text{H}$, and $\text{As}+3\text{H}$ surface species. Comparison with earlier $\text{PH}_3/\text{Si}(001)$ calculations [2] reveals that the relative stability of phosphine and arsine species is qualitatively the same. There are, however, some differences in the activation energies between these two systems that affect in significant ways the rate of dissociation and the preferred path taken. We relate these findings to available experimental observations. [1] M. Fuechsle, J.A. Miwa, S. Mahapatra, H. Ryu, S. Lee, O. Warschkow, L.C.L. Hollenberg, G. Klimeck, and M.Y. Simmons, *Nature Nanotechnology* 7, 242246 (2012). [2] O. Warschkow, N.J. Curson, S.R. Schofield, N.A. Marks, H.F. Wilson, M.W. Radny, P.V. Smith, T.C.G. Reusch, D.R. McKenzie, and M.Y. Simmons, *J. Chem. Phys.* 144 (2016) 014705.

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