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**The diffusion pathways of phosphorus atoms in the silicon (001) surface** JENNIFER BENNETT, OLIVER WARSCHKOW, Centre for Quantum Computer Technology, School of Physics, The University of Sydney, NIGEL MARKS, Nanochemistry Research Institute, Curtin University of Technology, DAVID MCKENZIE, Centre for Quantum Computer Technology, School of Physics, The University of Sydney — Effective use of surface chemical reactions to control the placement of dopants in semiconductors requires a detailed understanding of the reaction pathways involved. The most highly developed approach to accurate placement of phosphorus in silicon involves reacting phosphine gas with selected areas of the silicon (001) surface, incorporating the phosphorus atom into the surface and silicon overgrowth. In this computational study we investigate the least understood chemical reactions involved in this process, namely the phosphorus incorporation and associated diffusion reactions. We use density functional theory, combined with an efficient method for locating transition states, to identify the reaction pathways involved in three processes: (1) the diffusion of a phosphorus adatom along the silicon (001) surface, (2) the incorporation of a phosphorus atom into the surface, and (3) the migration of the incorporated phosphorus atom within the surface. The calculated pathways and corresponding reaction barriers provide insight into the conditions required for accurate incorporation and encapsulation of phosphorus atoms into the silicon surface.

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