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Determining exact location of Group V dopants below the Si(001):H surface from scanning tunnelling spectroscopy and density functional theory[1] VERONIKA BRAZDOVA, KITIPHAT SINTHIPTHARAKOON, PHILIPP STUDER, DAVID R. BOWLER, ADAM RAHNEJAT, NEIL J. CURSON, STEVEN SCHOFIELD, ANDREW J. FISHER, University College London — Group V impurities in silicon provide a way to tailor properties of electronic materials. The magnetically quiet environment that silicon provides for the impurity spins has also lead to new applications in coherent quantum devices. In both the ultimate classical devices and in future quantum computers the exact position of the dopants near surfaces and interfaces will determine the functionality: the ability to control and monitor those positions is key in these technologies. We precisely determine the substitutional sites of neutral As dopants that lie between 4.2 A and 15.0 A below the hydrogenated Si(001) surface, using a combination of density functional theory and low-temperature scanning tunnelling microscopy. We describe the interaction of the donor-electron state with the surface.

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