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Electronic Structure Models of Phosphorus Delta-Doped Silicon OLIVER WARSCHKOW, DAMIEN J. CARTER, Centre for Quantum Computer Technology, School of Physics, The University of Sydney, NIGEL A. MARKS, Nanochemistry Research Institute, Curtin University of Technology, DAVID R. MCKENZIE, Centre for Quantum Computer Technology, School of Physics, The University of Sydney — We report a full density functional theory treatment of phosphorus delta-doped silicon. A particular difficulty of this system is associated with the large delocalization lenghts of donor electrons in the host. To this end, we use large asymmetric unit cells with up to 800 atoms, and we obtain first-principles doping potentials, band energies and donor electron distributions. We additionally examine the electronic effects of overlapping doping potentials when two delta-doped planes are bought into proximity.

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