

Abstract Submitted
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A study of doped semiconducting nanowires using linear-scaling density-functional theory FABIANO CORSETTI, ARASH A. MOSTOFI, Thomas Young Centre, Imperial College London — In recent years, the possibility of using semiconducting nanowires as building blocks for future nanoscale devices has generated considerable interest in understanding and theoretically predicting the effect of point defects in such structures. To this end, we present a fully *ab initio* study of both the neutral vacancy and gold substitutional defect in bulk silicon and SiNWs. We follow a systematic methodology for converging the defect formation energy using the supercell approach within plane-wave DFT [1]. Our results highlight the importance of using large supercells to accurately describe the long-ranged disturbance effects caused by point defects in crystal lattices. We show that the linear-scaling DFT code ONETEP [2] can be used to study defects in large systems with thousands of atoms without loss of accuracy, thereby allowing calculations on realistically sized NWs. We also compute maximally localized Wannier functions for the defect systems; these provide insight into the nature of the electronic bonds that are formed between atoms in the vicinity of the defect. Finally, we discuss phonon calculations on defect centres using ONETEP to determine the thermodynamic properties of these systems. [1] M. J. Probert and M. C. Payne, Phys. Rev. B **67**, 075204 (2003). [2] C.-K. Skylaris, P. D. Haynes, A. A. Mostofi, and M. C. Payne, J. Chem. Phys. **122**, 084119 (2005).

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