

Abstract Submitted  
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**The electronic structure of Group V dopants in silicon – The requirements for a realistic DFT model**<sup>1</sup> VERONIKA BRAZDOVA, DAVID R. BOWLER, ANDREW J. FISHER, University College London — Typical concentrations of Group V donors in Si wafers used in experiment are up to  $10^{18} \text{ cm}^{-3}$ . In contrast, the simulation cell in a typical atomistic simulation would contain a few hundred Si atoms and one or two dopants. That is equivalent to concentrations on the order of at least  $10^{20} \text{ cm}^{-3}$ . We investigate the effect of donor concentration on the electronic structure of doped bulk silicon in density functional simulations (DFT) using the linear scaling DFT code Conquest on very large cells, and the cell sizes required to model the metal-semiconductor transition correctly.

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