

Spin-polarised first principles study of short dangling bond wires on the silicon (001) surface

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Short (2-5 atoms long) dangling bond wires, fabricated on H-terminated Si(001) surfaces, show patterns of Jahn-Teller effect induced displacement that depend on their length. In order to investigate the atomic and electronic structure, we performed density function calculations using VASP (2x2x1 k -points, 200eV cutoff), with and without spin-polarisation, on an 8 dimer long, 1 dimer wide and 6 layer deep cell for the wire lengths above and also for both an infinite wire and a saturated surface.

We find that our results from spin-polarised simulations are in good agreement with experimental observations. In particular, we find that the final displacements obtained for short odd-length wires are much smaller with spin than without spin. The results obtained with spin in odd-length wires are also in much better agreement with experiment. For even-length wires, good agreement is obtained regardless of whether spin is used or not.