

Abstract Submitted
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Magnetism in Cr doped Si nanowires MICHAEL SHAUGHNESSY,
UC Davis/ LLNL, C.Y. FONG, UC Davis, LIN YANG, LLNL — We carry out first
principles calculations of magnetic and electronic structures of single and multiple
Cr atom dopants in Si nanowires. Both unsupported isolated wires and supported
wires on Si 110 surfaces are studied. The relative stability and underlying physical
picture of the ferromagnetic and antiferromagnetic configurations of the local mo-
ments on the Cr atoms are studied. Results are also presented for fully noncollinear
calculations.

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