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 moments on the Cr atoms are studied. Results are also presented for fully noncollinear calculations.