Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

V, Nb and Ta doping of anatase TiO_2: from a dilute magnetic semiconductor to a transparent conducting oxide[1] JORGE OSORIO-GUILLÉN, STEPHAN LANY, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO 80401 — We have investigated by means of first-principle supercell calculations the effects of doping anatase TiO_2 by V, Nb and Ta. We find: (*i*) V doping makes TiO_2:V ferromagnetic. A single V impurity has a magnetic moment of 1.0 μ_B/V atom with an electronic configuration $a_1^2\, t_{1+}^3\, t_{1-}^3\, t_{2+}^1\, t_{2-}^0\, e_+^0\, e_-^0$. The ferromagnetic interaction between two V impurities is found to extend to more than fifth neighbors, with calculated ferromagnetic stabilization energy raging from 124 meV at the first neighbor to 27 meV at the fifth neighbor. (*ii*) Nb and Ta doping of TiO_2 makes the system conductive, but not magnetic. The calculated equilibrium free-electron concentration (n_e) at $T = 1000$K for Ti-rich–O-poor growth conditions is 2.7×10^{21} and 5.9×10^{21} cm^{-3} for Nb and Ta doping respectively, whereas pure TiO_2 is calculated to have a electron density of only 1.8×10^{18} cm^{-3} due to intrinsic defects. Thus, Nb and Ta doping of TiO_2 enhance dramatically the electron concentration and hence are good transparent conductor oxides.

[1]This work was funded by DARPA under NREL contract No. DE-AC36-99GO10337

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Date submitted: 20 Nov 2006 Electronic form version 1.4