V, Nb and Ta doping of anatase TiO$_2$: from a dilute magnetic semiconductor to a transparent conducting oxide\textsuperscript{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 $\mu_B$/V atom with an electronic configuration $a^2 t_{1g}^3 t_{2g}^1 t_{3g}^1 e_0^0 e_0^-$. The ferromagnetic interaction between two V impurities is found to extend to more than fifth neighbors, with calculated ferromagnetic stabilization energy ranging 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 $2.7 \times 10^{21}$ and $5.9 \times 10^{21}$ cm$^{-3}$ for Nb and Ta doping respectively, whereas pure TiO$_2$ is calculated to have an electron density of only $1.8 \times 10^{18}$ 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.

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