Appendix A Paramagnetic bands in the Brillouin zone

A possible explanation of the unusual magnetic moment of $Ti_{23}CuO_{48}$ can be found in Fig. A1 showing the spin-polarized bands in the Brillouin Zone. Close examination of the curves under the Fermi level shows lower energy (larger population) for the spin-up states in the branches $\Gamma - M$ and $\Gamma - X$ of the diagram. Then, there will be more spin-up states populating than spin-down states, thus yielding a net difference and a magnetic moment for the system.

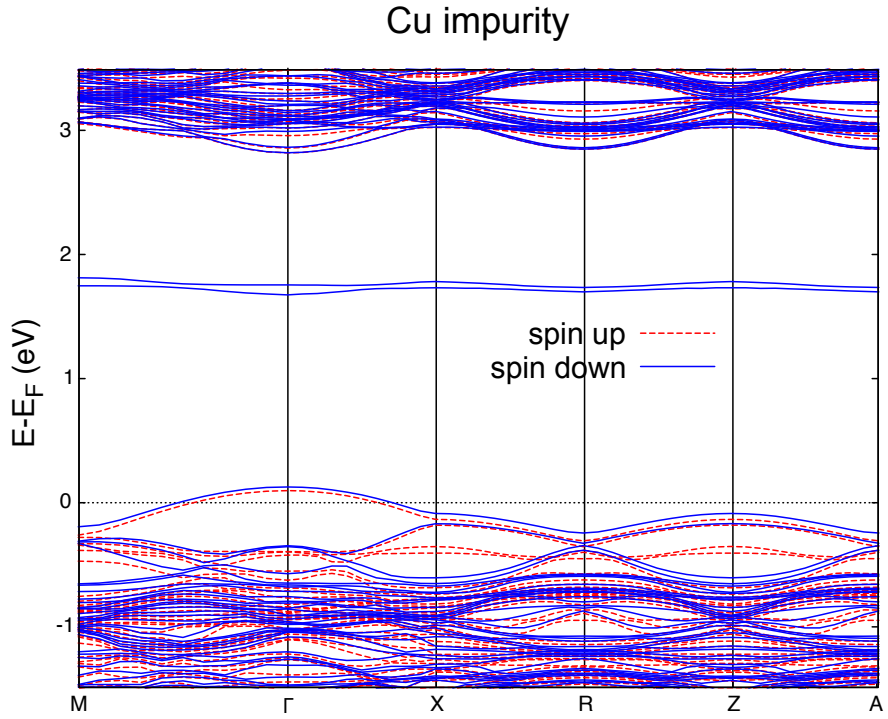

Fig. A1 Band structure for the spin-polarized case of $Ti_{23}CuO_{48}$.

Appendix B Spin-polarized density of states

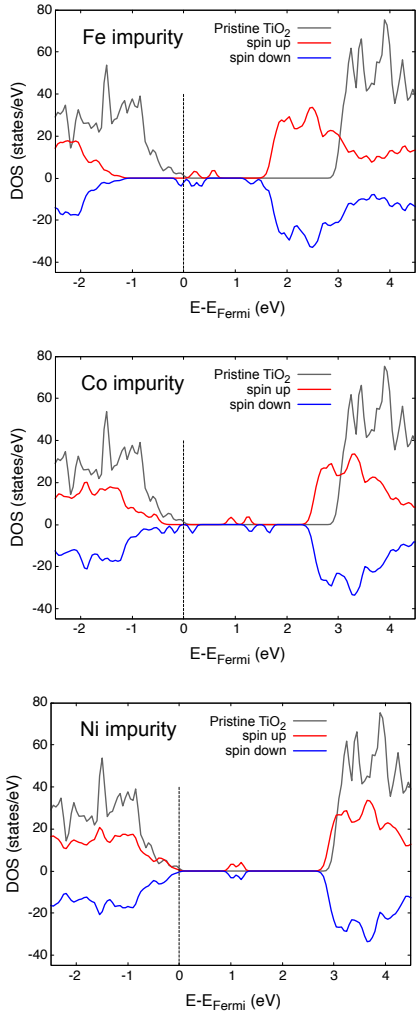

Fig. B2 Spin-polarized density of states for $Ti_{23}AO_{48}$: A = Fe (upper panel); A = Co (middle panel) and A = Ni (bottom panel). The DOS for pristine TiO_2 is plotted in dashed line in each case.

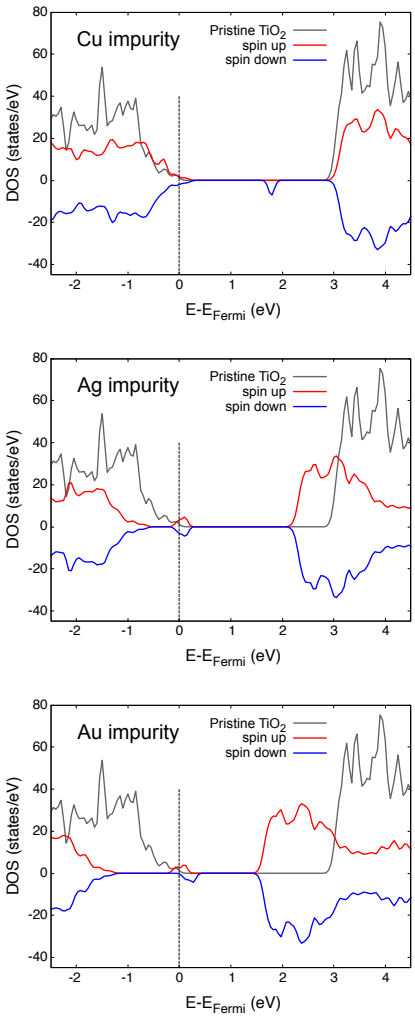

Fig. B3 Spin-polarized density of states for $Ti_{23}AO_{48}$: A = Cu (upper panel); A = Ag (middle); A = Au (bottom panel). The DOS for pristine TiO_2 is plotted in grey line in each case.

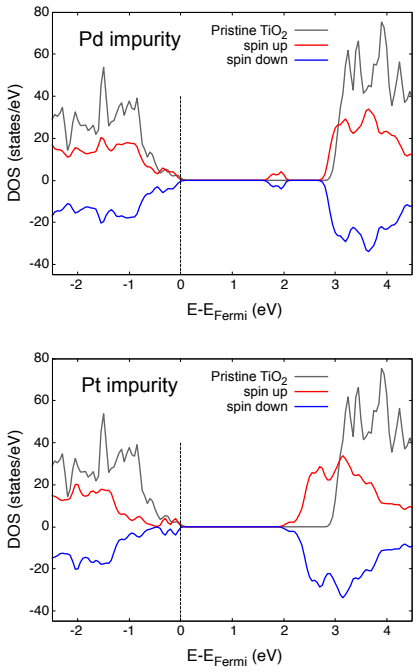

Fig. B4 Spin-polarized density of states for $Ti_{23}AO_{48}$: A = Pd (upper panel); A = Pt (bottom panel). The DOS for pristine TiO_2 is plotted in grey line in each case.