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Supplementary Information: Substitutional 4d and 5d Impurities in Graphene†

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Projected density of states

Figure 1 shows the projected density of states for graphene with an impurity of the elements from the chromium and manganese groups. As commented in the article, the total magnetic moment for graphene with an impurity of the manganese group depends on the filling of a majority A symmetry level or a minority E symmetry level. Those levels are marked with green ellipses in Fig. 1. For 4d and 5d elements the reduced spin splitting yields the possibility of filling minority E symmetry level first for technetium and rhenium cases. This causes the reduction of the total magnetic moment from 3 to $1\mu_B$ for technetium and rhenium cases.

Figure 2 shows also the projected density of states for graphene and an impurity of the nine elements in the iron, cobalt and nickel groups. First of all, notice the similarity of the electronic structure between 4d and 5d, as commented above for the chromium and manganese groups. The projected density of states follows a similar pattern for the couples of ruthenium osmium, rhodium iridium and palladium platinum, while it is slightly different for iron, cobalt and nickel respectively. Nevertheless, close to the Fermi energy, all the elements in the these groups seem equally. For the iron group there is spin compensation and the LUMO levels with either spin up or down have A symmetry. Moving to the cobalt group, the spin majority A symmetry level becomes occupied, giving rise to the already commented total cell magnetic moment of $1\mu_B$. Logically, for the nickel group the addition of another electron fills the minority A symmetry level, depleting the total magnetic moment. Those important A symmetry levels are marked up with green ellipses in the upper panels of in Fig. 2.

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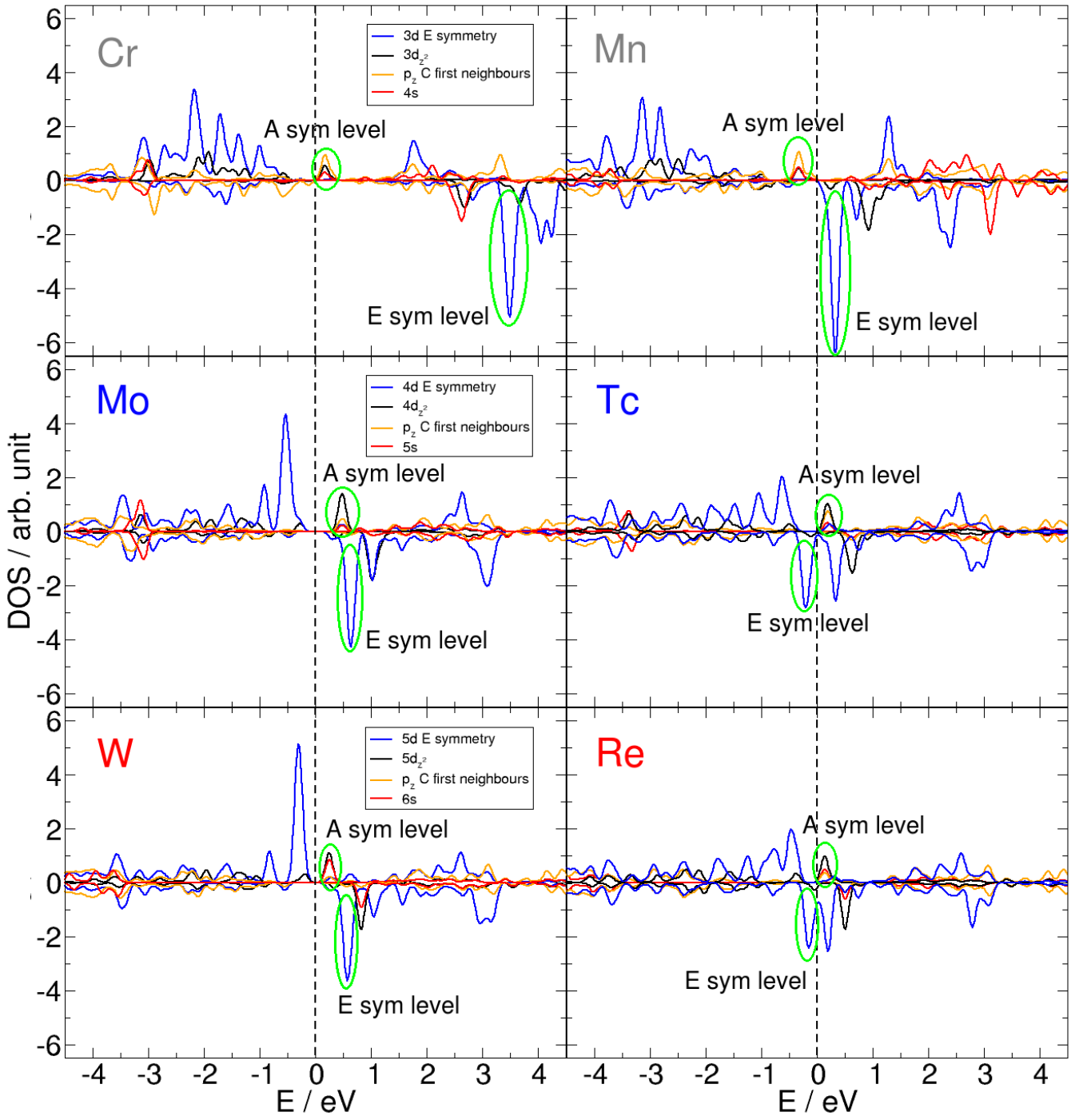

Fig. 1 Projected density of states of graphene with the impurities of chromium and manganese groups. The element of the impurity in graphene is labelled for each graph. Green ellipses denote the A and E symmetry levels, which are key to understand the reduction of the total magnetic moment between the technetium and manganese cases.

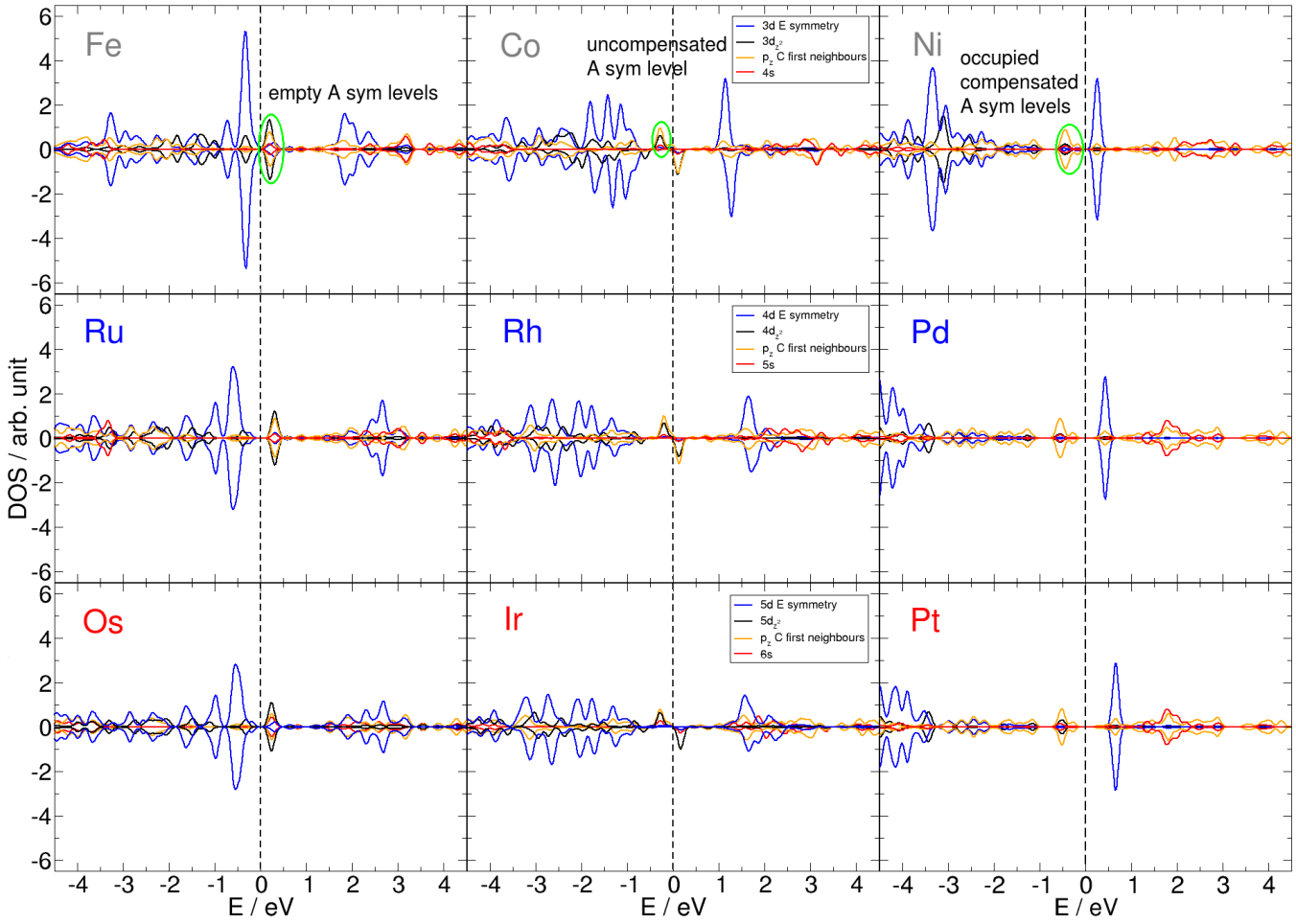

Fig. 2 Projected density of states of graphene with the impurities of iron, cobalt and nickel groups: the element is labelled for each graph. Green ellipses denote A symmetry levels, which are key to understand the evolution of the total magnetic moment within these three groups.