Journal Name

ARTICLE TYPE

Supplementary Information

Individual atomic Magnetic Moments

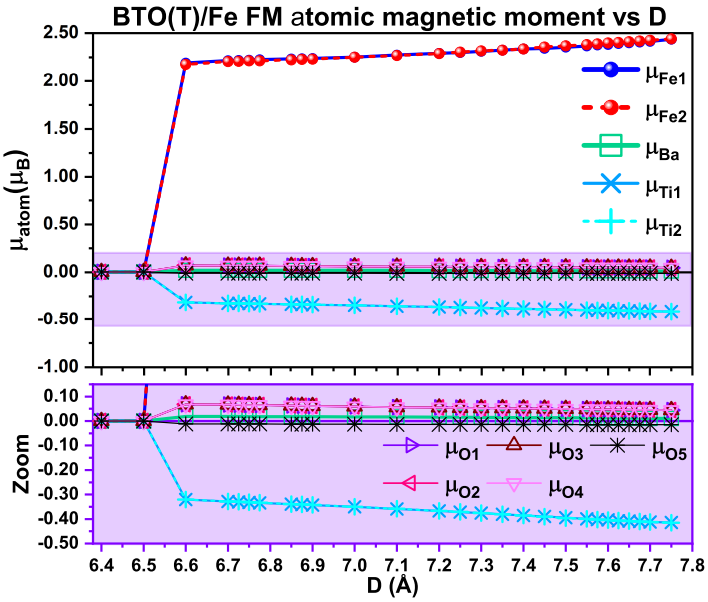

Fig. S1 Individual atomic magnetic moments for the ferromagnetic alignment of BTO(T)/Fe supercell.

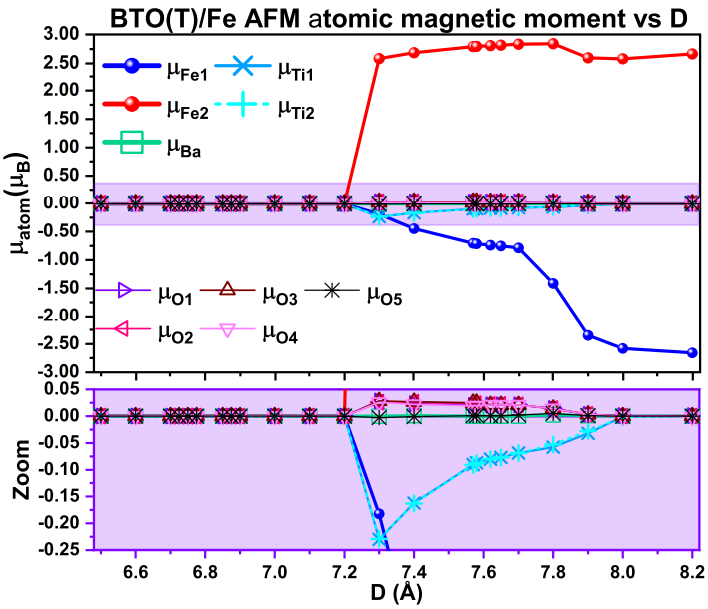

Fig. S2 Individual atomic magnetic moments for the antiferromagnetic alignment of BTO(T)/Fe supercell.

[a] *Physics Department and CICECO, University of Aveiro, 3810-193 Aveiro, Portugal; E-mail:amorim5@ua.pt*

† Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/b000000x/

Total and Spin Polarised Charge Density

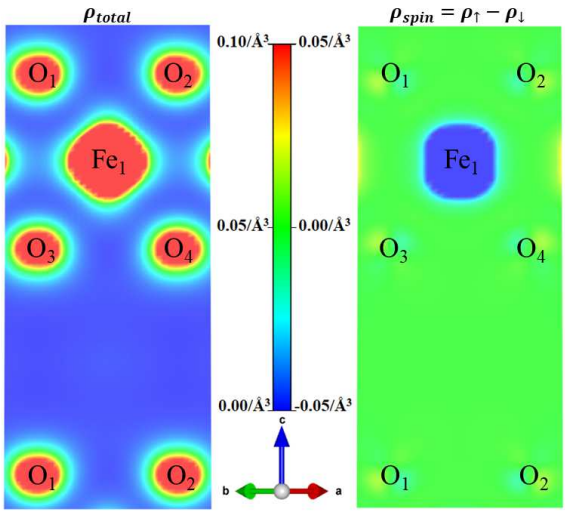

Fig. S3 Charge density (left) and SP charge density difference (right) of the AFM state for **D** $= 8.1$ Å, across plane A, calculated for $E - E_F \in [-3.75, 0]$ eV.

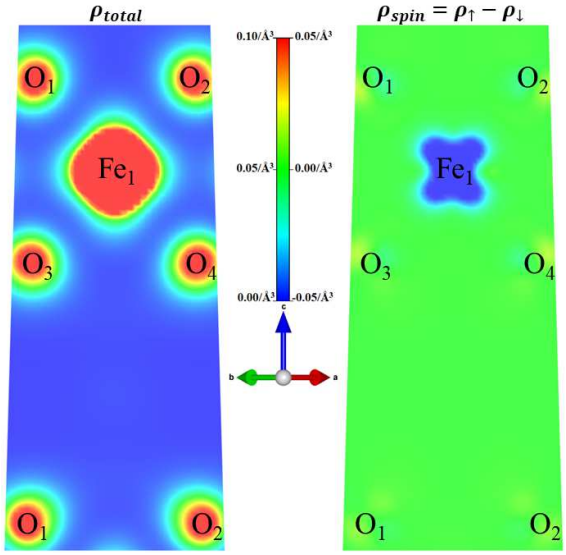

Fig. S4 Charge density (left) and SP charge density difference (right) of the FiM state for **D** $= 7.5$ Å, across plane A, calculated for $E - E_F \in [-3.75, 0]$ eV.

DOS comparison

To have a clearer comparison between the DOS of each magnetic state, the total DOS and Fe DOS of figures **??**,**??**, **??** and **??** were merged into figure S5.

It is possible to see that the DOS of the Fe2 atom of the FiM state is quite similar to the Fe1 and Fe2 DOS of the FM state, with local maxima with similar location and relative intensities. The same does not happen with the Fe1 of the FiM state which has an anti-parallel magnetic moments with lower magnitude.

On the other hand, the AFM and NS states have qualitatively different DOS from the FiM and FM states, (and between them) for both the Fe1 and Fe2 cases.

Another interesting features is that, while the FM, FiM and AFM states have DOS of a metallic or semimetallic nature, the NS state possesses a small band gap (of about 200 meV).

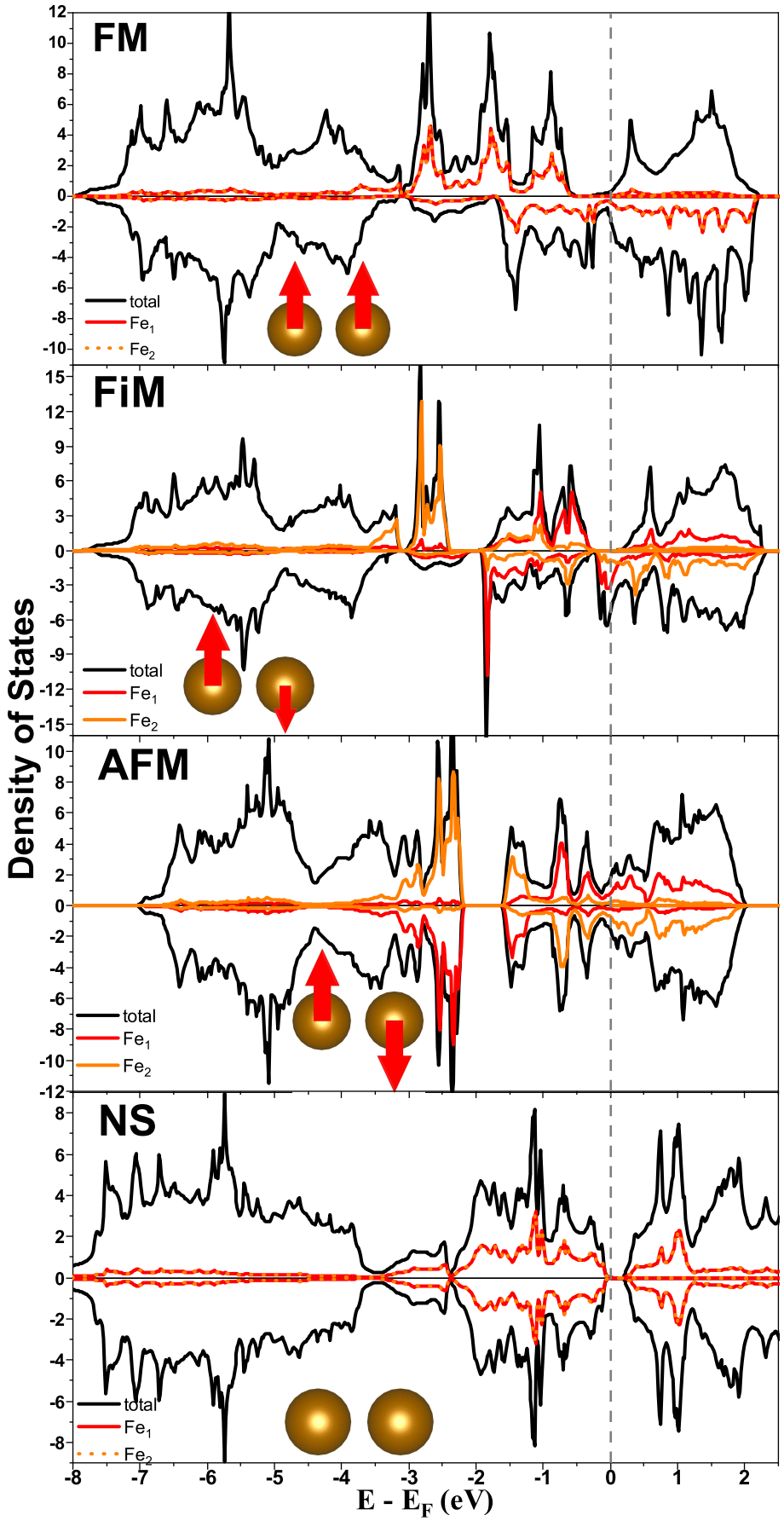

Fig. S5 Comparison between DOS of all magnetic states presented in the current manuscript. From top to bottom: FM, FiM, AFM and NS states, respectively.