Electronic and magnetic properties of Fe clusters inside finite zigzag single wall carbon nanotubes

Supplemental Material

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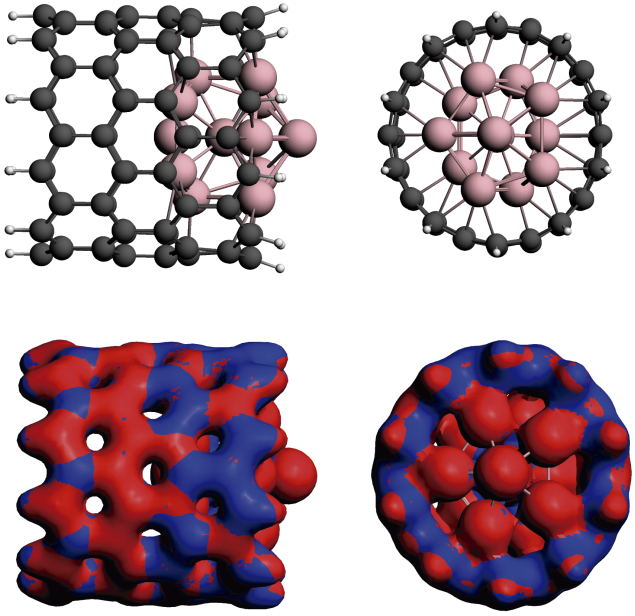

FIG. 1: (Color online) Lateral and front views of the equilibrium structure of icosahedral Fe_{12} encapsulated inside a short $(10,0)$ ZNT, and of the corresponding spin density. The isosurfaces for the spin densities correspond to $\rho_\alpha(\vec{r}) = 0.025\ a.u.$ (red) and $\rho_\beta(\vec{r}) = 0.025\ a.u.$ (blue). The surface shown corresponds to the most external one, then a red (blue) color indicates that the atoms have excess $\alpha(\beta)$ population.

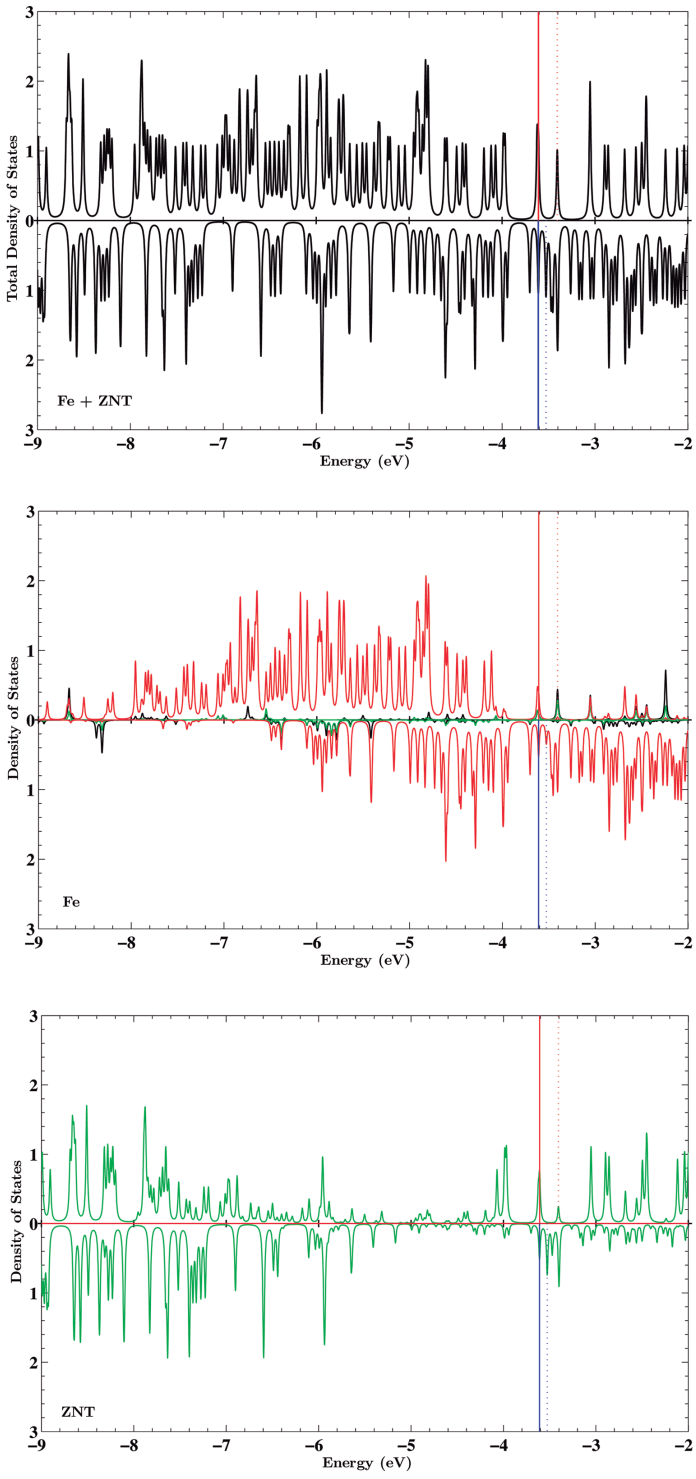

FIG. 2: (Color online) Electronic density of states, in arbitrary units, for icosahedral Fe_{12} encapsulated inside a short $(10, 0)$ ZNT. The system is in its ground state, with total magnetic moment $\mu_T = 32\,\mu_B$. Upper panel: total DOS. Middle and lower panels: projections of the DOS on the Fe cluster and the nanotube, respectively. In each panel, upper curves correspond to majority spin states, and lower curves to minority spin. In the middle and lower panels, red curves stand for d character of the states, green curves for p, and black curves for s character. Vertical continuous lines indicate the position of the HOMO, and dashed lines the position of the LUMO. The states have been broadened with Lorenztians of width $\Gamma = 0.04\,\text{eV}$.

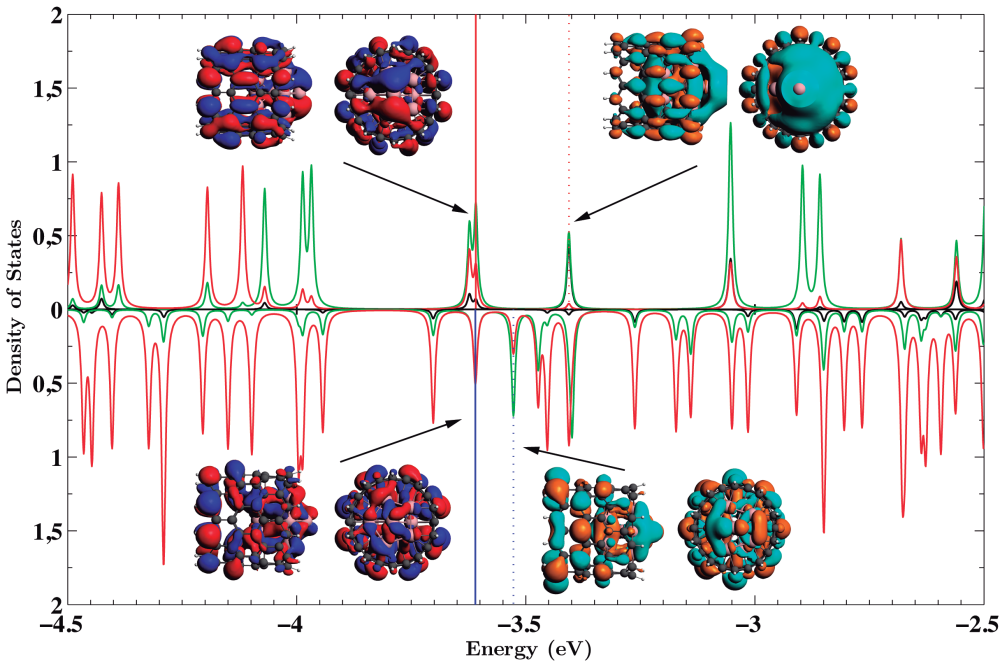

FIG. 3: (Color online) Expanded view of the total electronic density of states around the Fermi level for icosahedral Fe_{12} encapsulated inside a short $(10, 0)$ ZNT. The DOS is separated in s-like (black curves), p-like (green curves) and d-like (red curves) contributions. The Lorenztian width is $\Gamma = 0.01\,\mathrm{eV}$. Lateral and top views of the HOMO and LUMO orbitals are given in the insets.

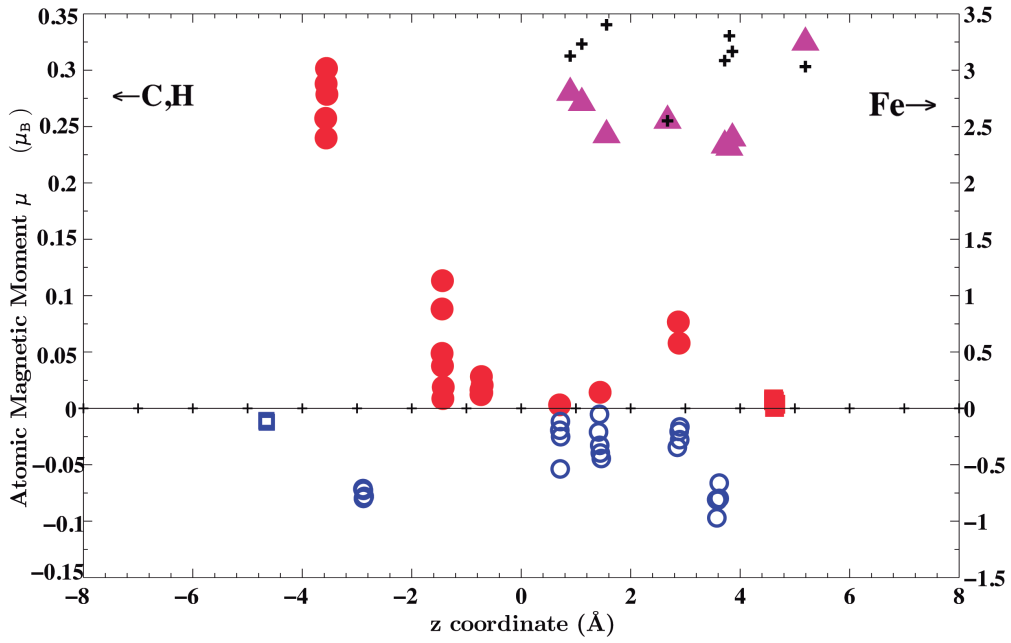

FIG. 4: (Color online) Atomic magnetic moments μ for icosahedral Fe_{12} encapsulated inside a short $(10, 0)$ ZNT as a function of the atom coordinate along the z axis of the nanotube. The atomic magnetic moments of the C (H) atoms with the same z coordinate vary with the position of the C (H) atoms on the ring. Triangles represent Fe atoms, circles represent C atoms (red circles, C atoms with dominant α spin character; blue circles, C atoms with dominant β spin character), and squares on the two ends represent H atoms. For comparison, the atomic magnetic moments of the free Fe_{12}-icosahedral cluster (crosses) are also shown. Note the different vertical scales for Fe (right) and for C (left).

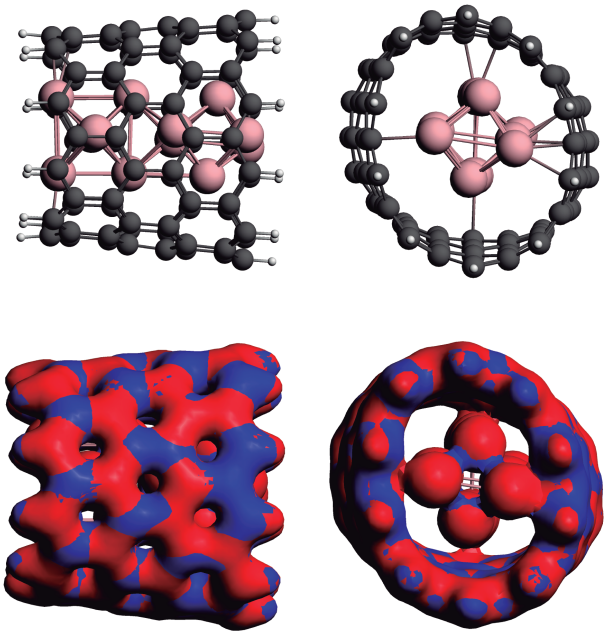

FIG. 5: (Color online) Lateral and front views of the equilibrium structure of an Fe_{12} tetrahedral chain encapsulated inside a short $(10, 0)$ ZNT, and of the corresponding spin density. The isosurfaces for the spin densities like in the caption of Figure 1 of this Supplemental Material.

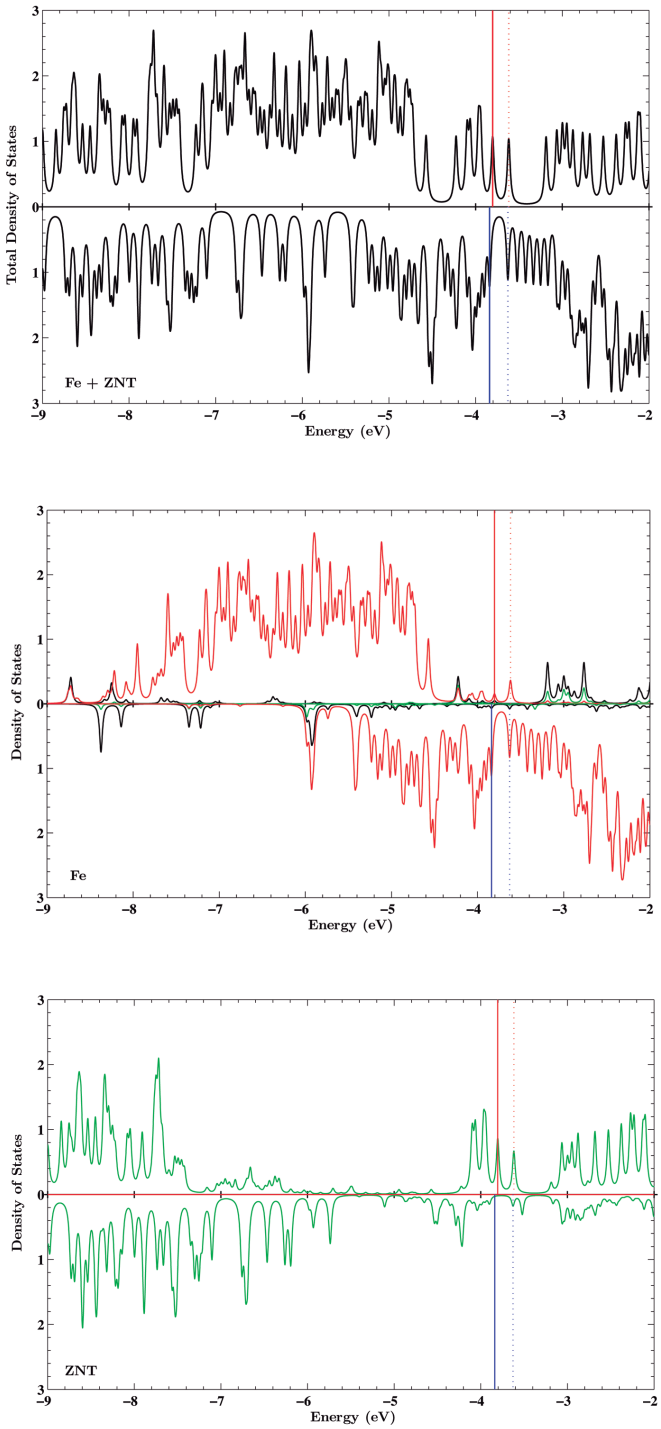

FIG. 6: (Color online) Electronic density of states, in arbitrary units, for an Fe_{12} tetrahedral chain encapsulated inside a short $(10, 0)$ ZNT. The system is in its ground state, with total magnetic moment $\mu_T = 34\,\mu_B$. See the caption of Figure 2 of this Supplemental Material.

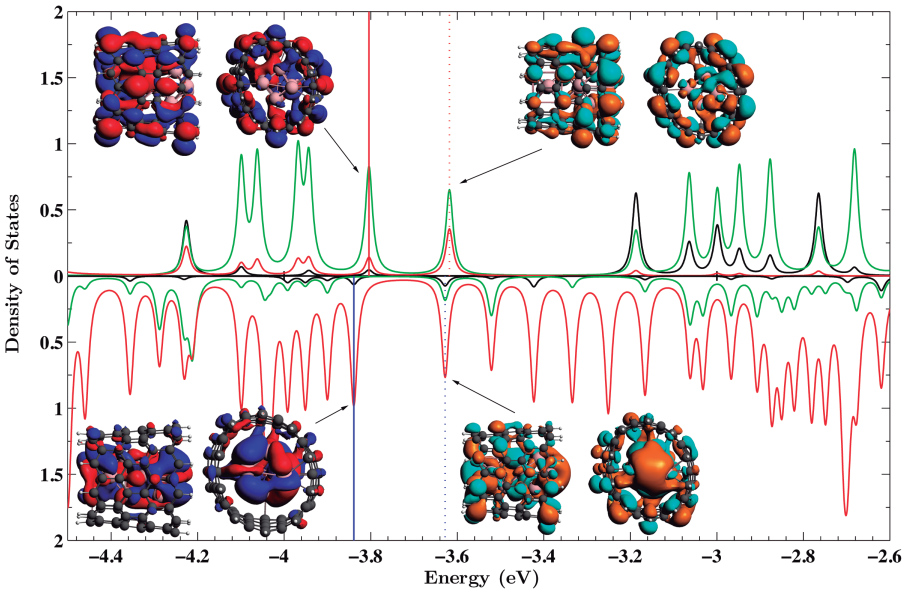

FIG. 7: (Color online) Expanded view of the total electronic density of states around the Fermi level for an Fe_{12} tetrahedral chain encapsulated inside a short $(10, 0)$ ZNT. The DOS is separated in *s*-like (black curves), *p*-like (green curves) and *d*-like (red curves) contributions. The Lorenztian width is $\Gamma = 0.01\,\text{eV}$. Lateral and top views of the HOMO and LUMO orbitals are given in the insets.

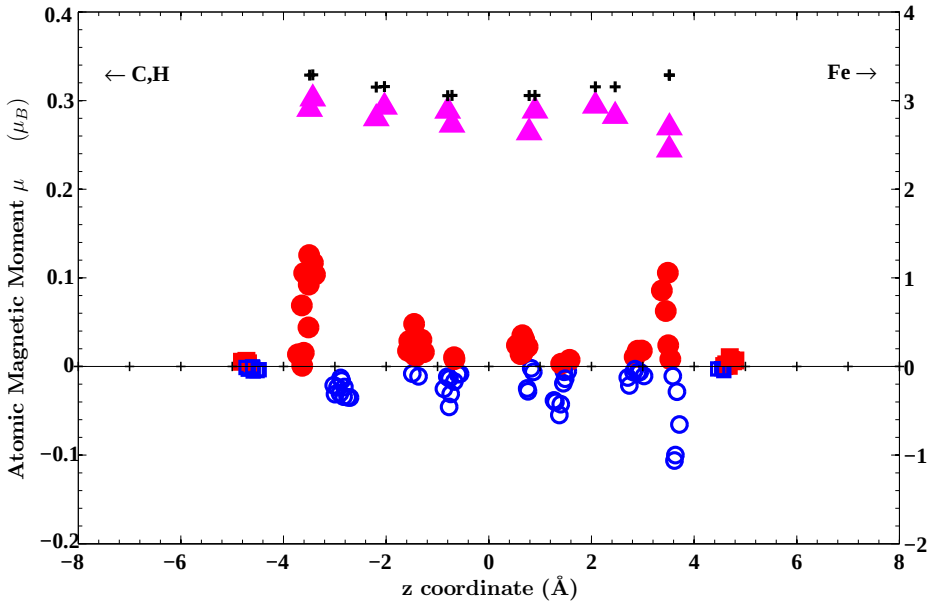

FIG. 8: (Color online) Atomic magnetic moments μ for an Fe_{12} tetrahedral chain encapsulated inside a short $(10, 0)$ ZNT as a function of the atom coordinate along the z axis of the nanotube. The atomic magnetic moments of the free Fe_{12}-tetrahedral chain (crosses) are also shown. Note the different vertical scales for Fe (right) and for C (left). See the caption of Figure 4 of this Supplemental Material.