Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

On the involvement of d-electrons in superatomic shells: the group 3 and 4 transition metals-Supplementary Material

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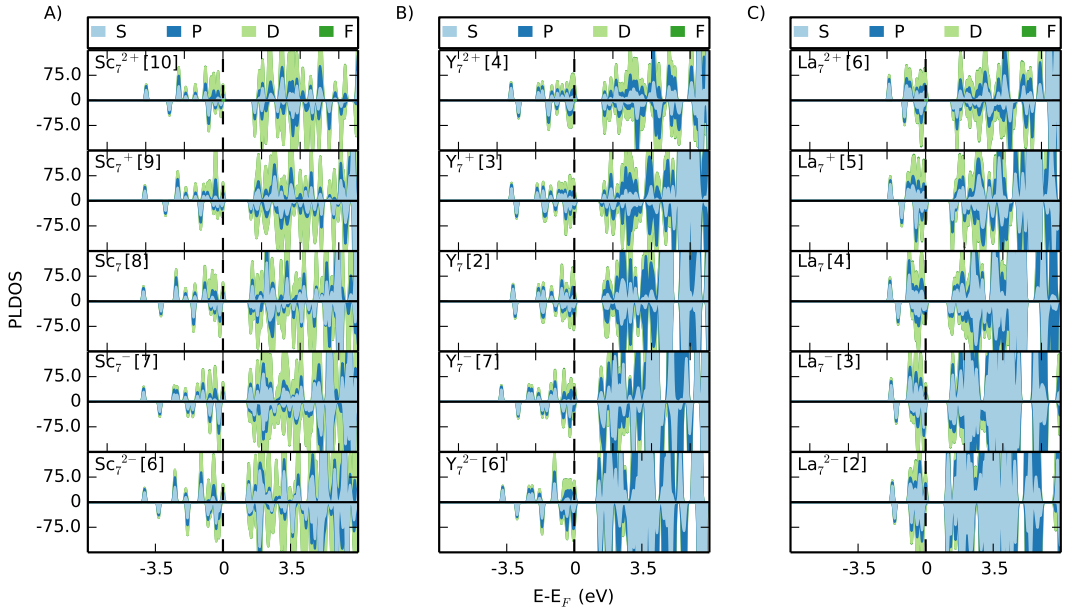

FIG. 1. Local angular momentum resolved density of states for the Sc_7, Y_7 and La_7 clusters, for the PBE0 exchange-correlation functional calculations, shown in subfigure A, B and C respectively. For each PLDOS the projection values are stacked on top of each other for the purpose of clarity. For each subfigure PLDOS images go down the page in increasing number of electrons. Presented in brackets on each PLDOS is the multiplicity of the cluster.

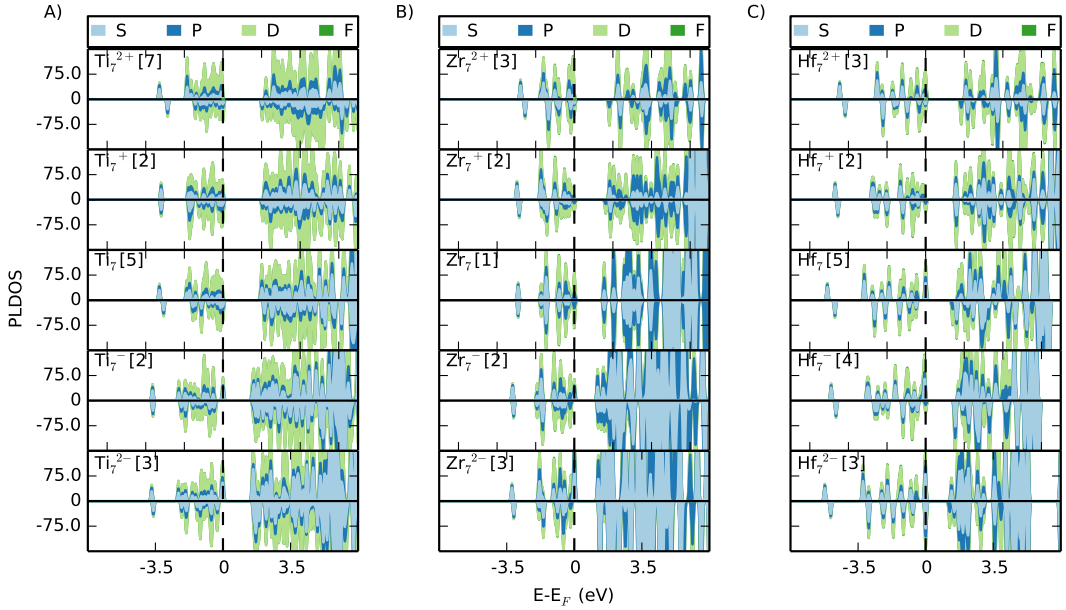

FIG. 2. Local angular momentum resolved density of states for the Ti_7, Zr_7 and Hf_7 clusters, for the PBE0 exchange-correlation functional calculations, shown in subfigure A, B and C respectively. For each PLDOS the projection values are stacked on top of each other for the purpose of clarity. For each subfigure PLDOS images go down the page in increasing number of electrons. Presented in brackets on each PLDOS is the multiplicity of the cluster.

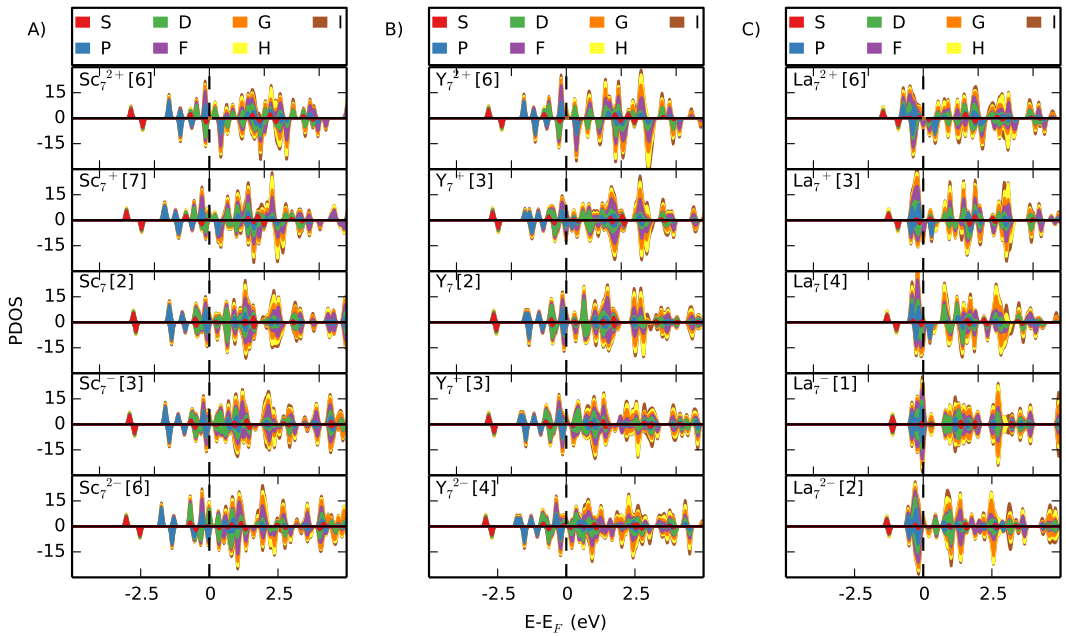

FIG. 3. Angular momentum resolved density of states for the Sc_7, Y_7 and La_7 clusters, for the PBE exchange-correlation functional calculations, shown in subfigure A, B and C respectively. For each PDOS the projection values are stacked on top of each other for the purpose of clarity. For each subfigure PDOS images go down the page in increasing number of electrons. Presented in brackets on each PDOS is the multiplicity of the cluster.

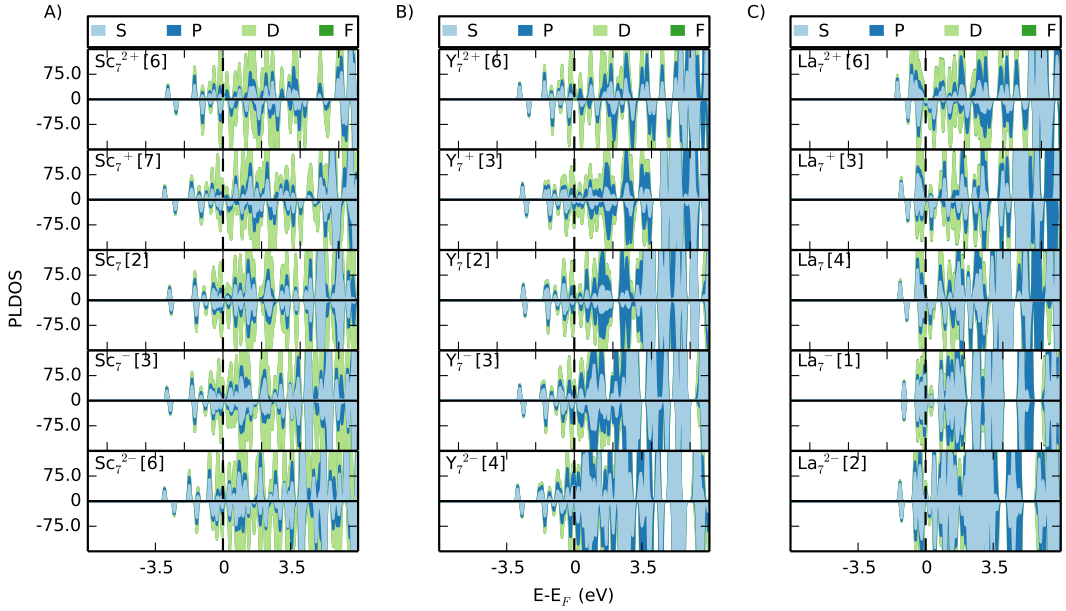

FIG. 4. Local angular momentum resolved density of states for the Sc_7, Y_7 and La_7 clusters, for the PBE exchange-correlation functional calculations, shown in subfigure A, B and C respectively. For each PLDOS the projection values are stacked on top of each other for the purpose of clarity. For each subfigure PLDOS images go down the page in increasing number of electrons. Presented in brackets on each PLDOS is the multiplicity of the cluster.

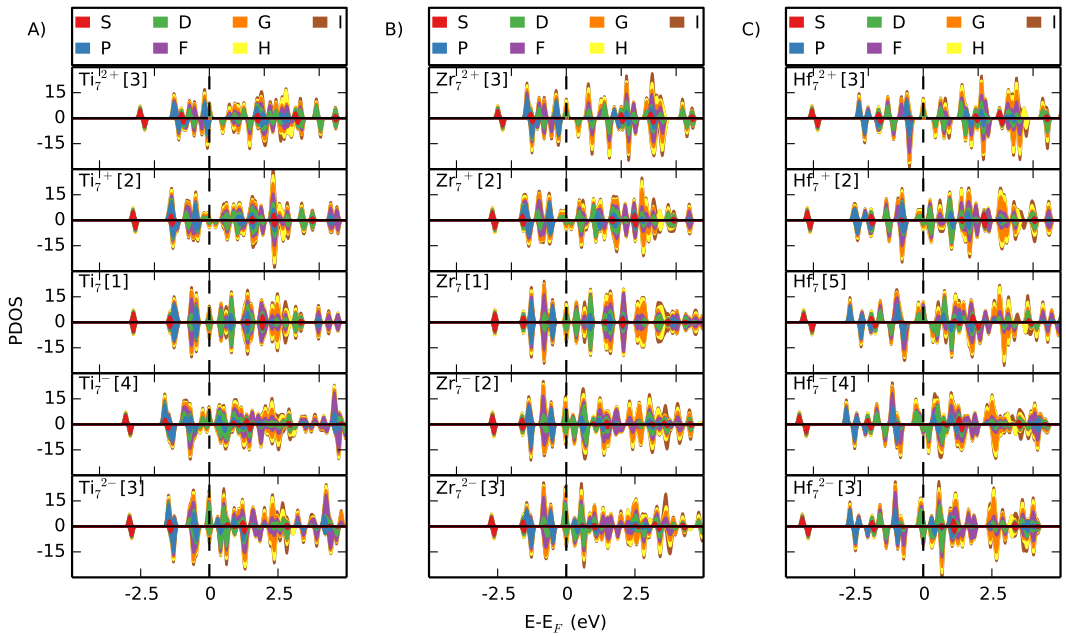

FIG. 5. Local angular momentum resolved density of states for the Ti_7, Zr_7 and Hf_7 clusters, for the PBE exchange-correlation functional calculations, shown in subfigure A, B and C respectively. For each PDOS the projection values are stacked on top of each other for the purpose of clarity. For each subfigure PLDOS images go down the page in increasing number of electrons. Presented in brackets on each PLDOS is the multiplicity of the cluster.

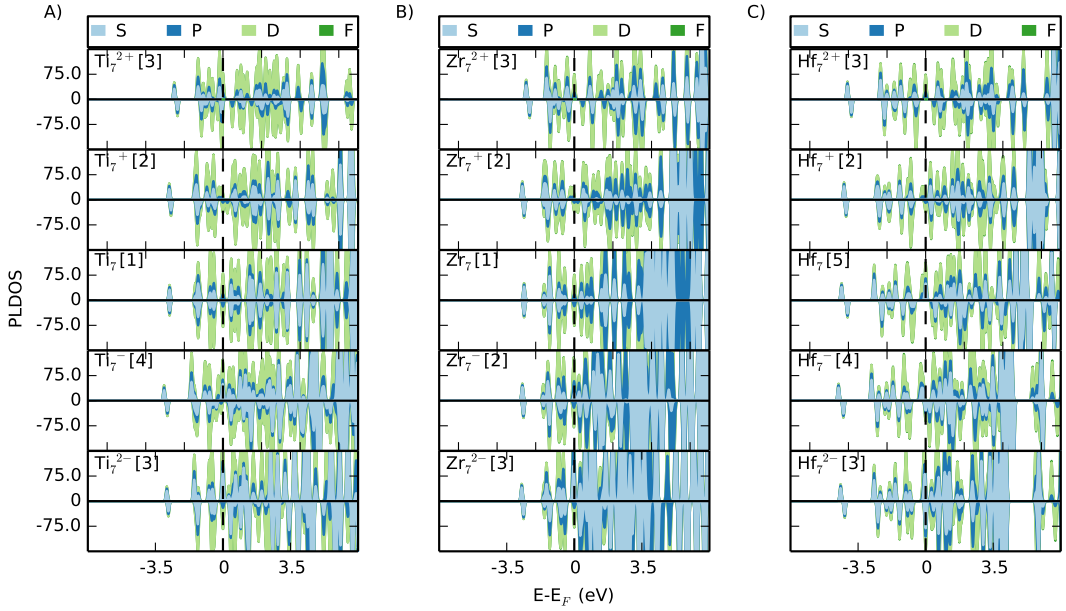

FIG. 6. Angular momentum resolved density of states for the Sc_7, Y_7 and La_7 clusters, for the PBE0 exchange-correlation functional calculations, shown in subfigure A, B and C respectively. For each PLDOS the projection values are stacked on top of each other for the purpose of clarity. For each subfigure PDOS images go down the page in increasing number of electrons. Presented in brackets on each PDOS is the multiplicity of the cluster.

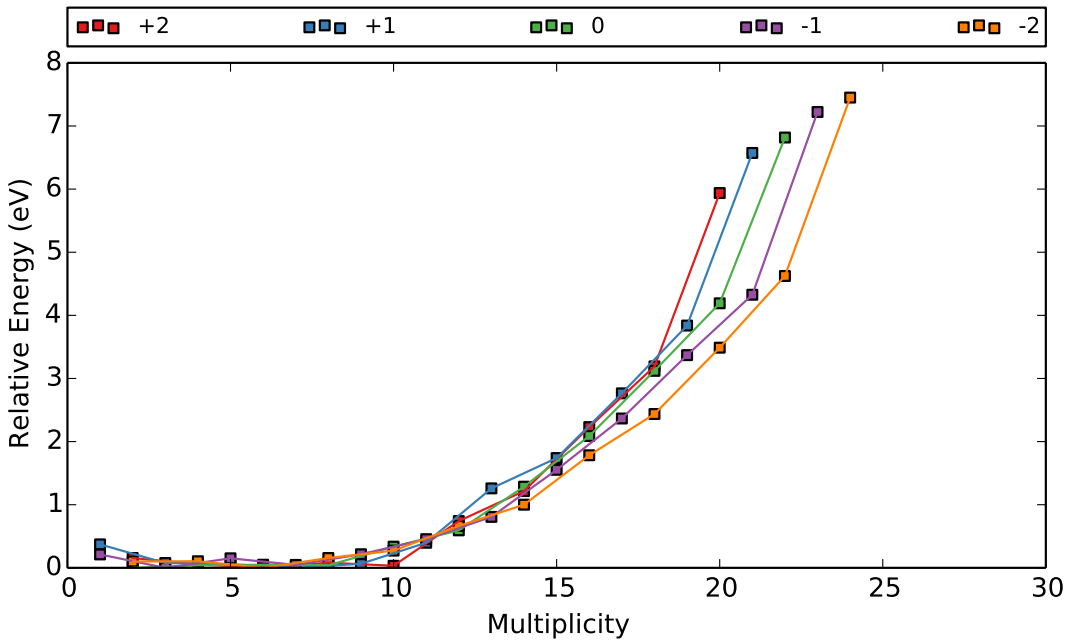

FIG. 7. Relative energies for the Scandium cluster calculations for the PBE functional at each multiplicity. The energies are all relative to the lowest energy for each charge state i.e. the ground state energy is set to 0.

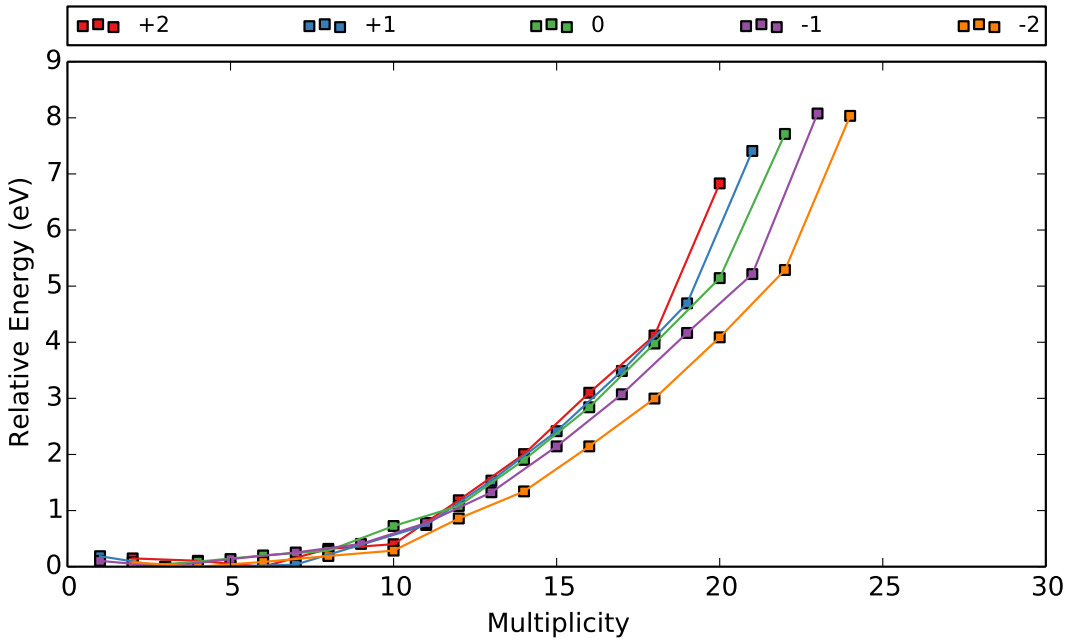

FIG. 8. Relative energies for the Yttrium cluster calculations for the PBE functional at each multiplicity. The energies are all relative to the lowest energy for each charge state i.e. the ground state energy is set to 0.

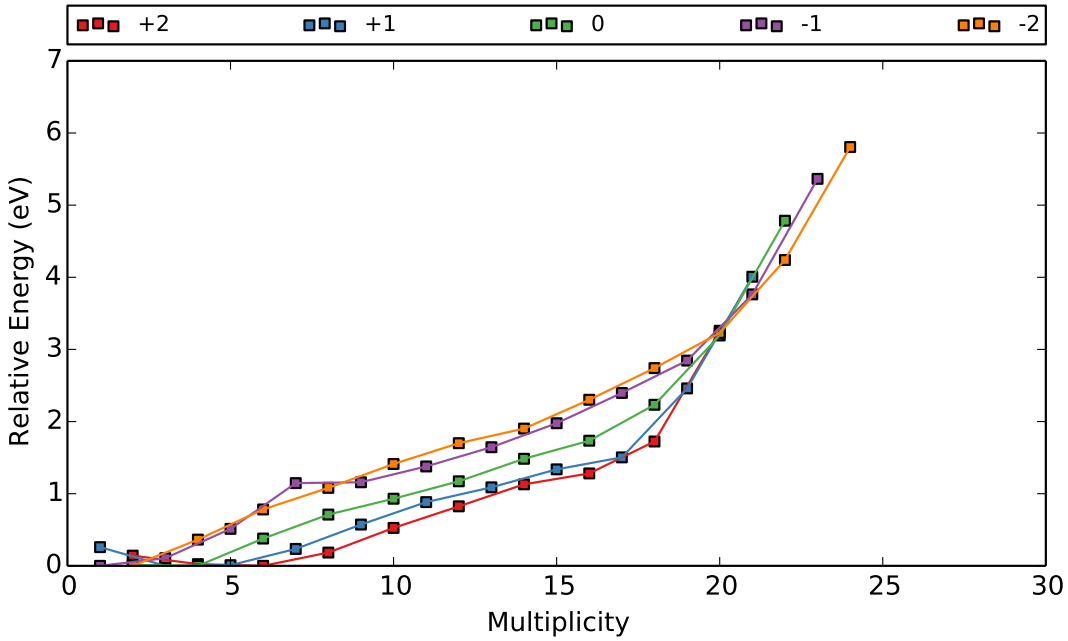

FIG. 9. Relative energies for the Lanthanum cluster calculations for the PBE functional at each multiplicity. The energies are all relative to the lowest energy for each charge state i.e. the ground state energy is set to 0.

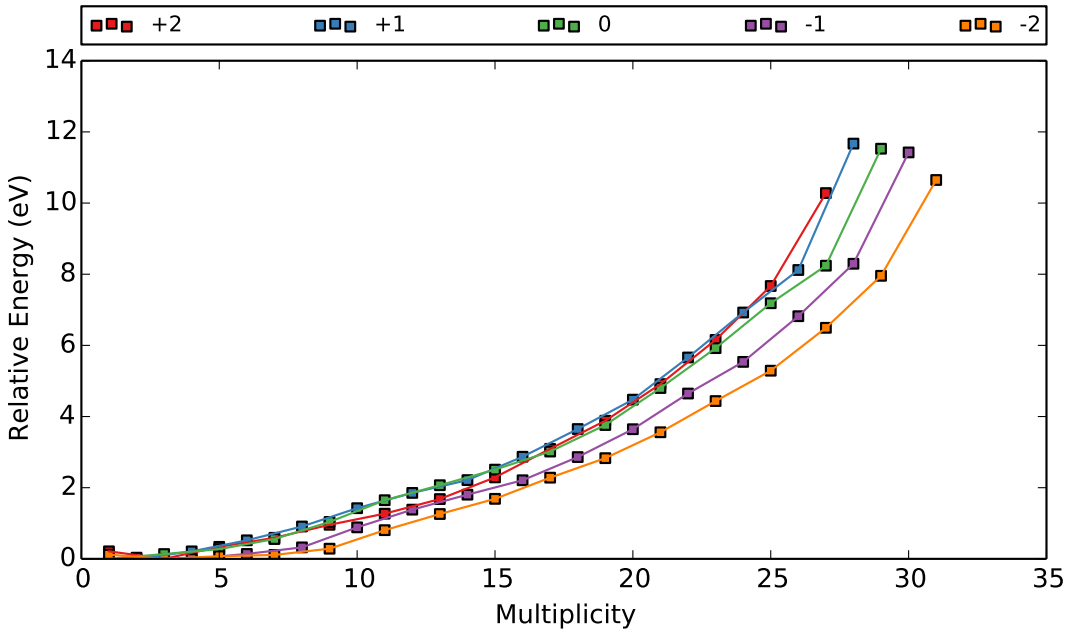

FIG. 10. Relative energies for the Titanium cluster calculations for the PBE functional at each multiplicity. The energies are all relative to the lowest energy for each charge state i.e. the ground state energy is set to 0.

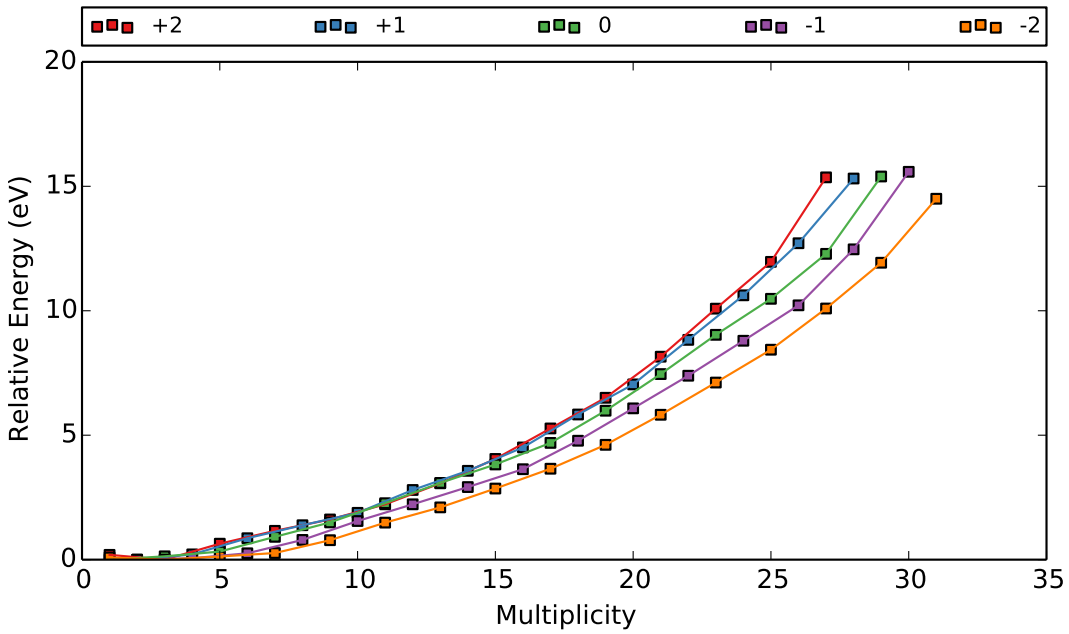

FIG. 11. Relative energies for the Zirconium cluster calculations for the PBE functional at each multiplicity. The energies are all relative to the lowest energy for each charge state i.e. the ground state energy is set to 0.

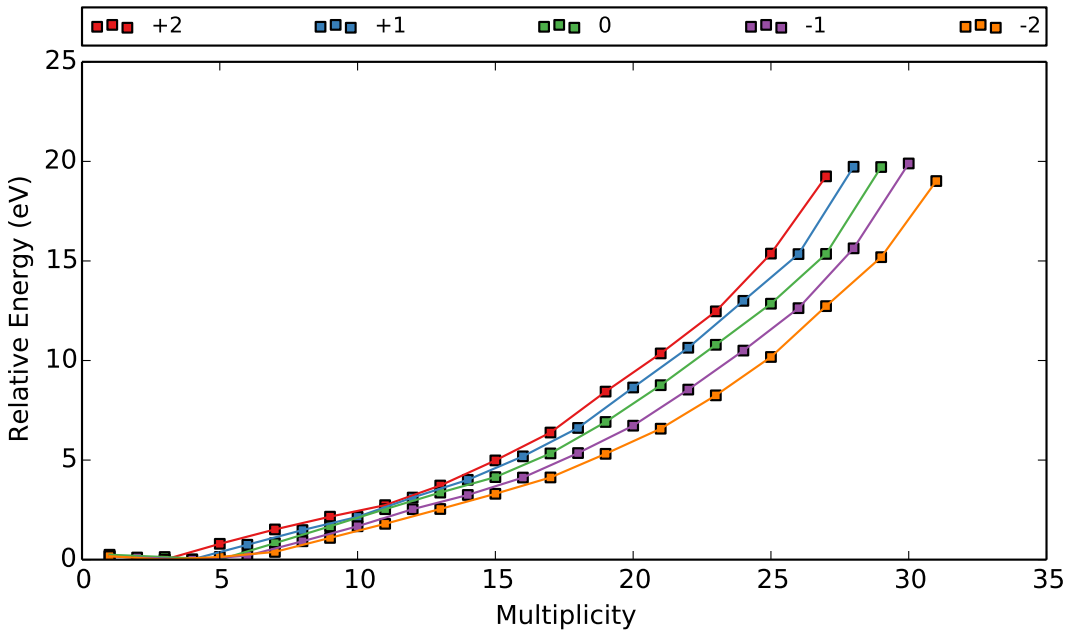

FIG. 12. Relative energies for the Hafnium cluster calculations for the PBE functional at each multiplicity. The energies are all relative to the lowest energy for each charge state i.e. the ground state energy is set to 0.

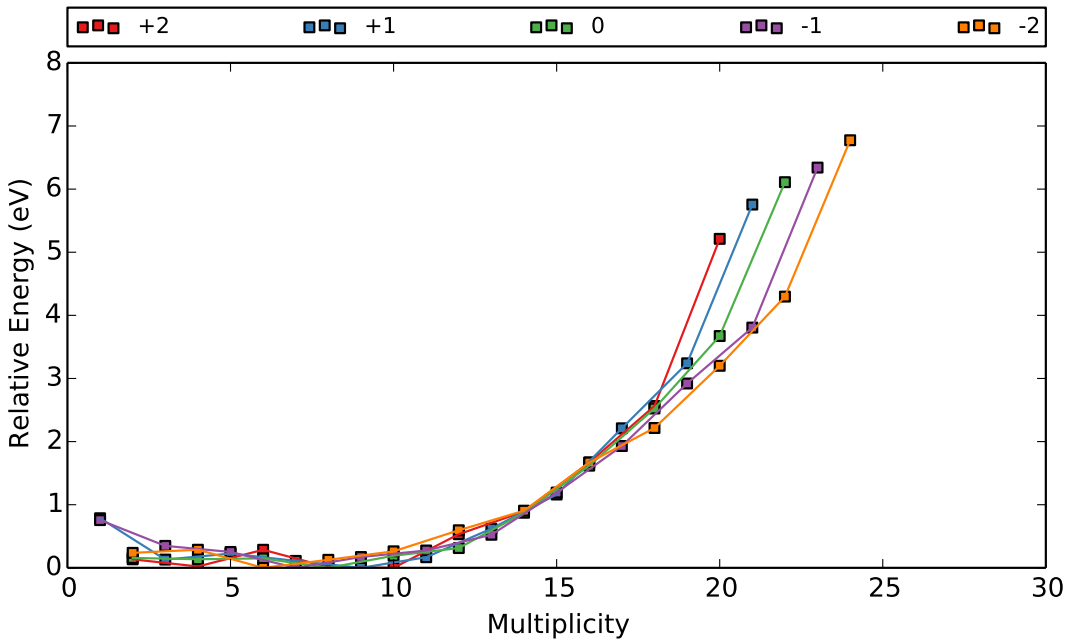

FIG. 13. Relative energies for the Scandium cluster calculations for the PBE0 functional at each multiplicity. The energies are all relative to the lowest energy for each charge state i.e. the ground state energy is set to 0.

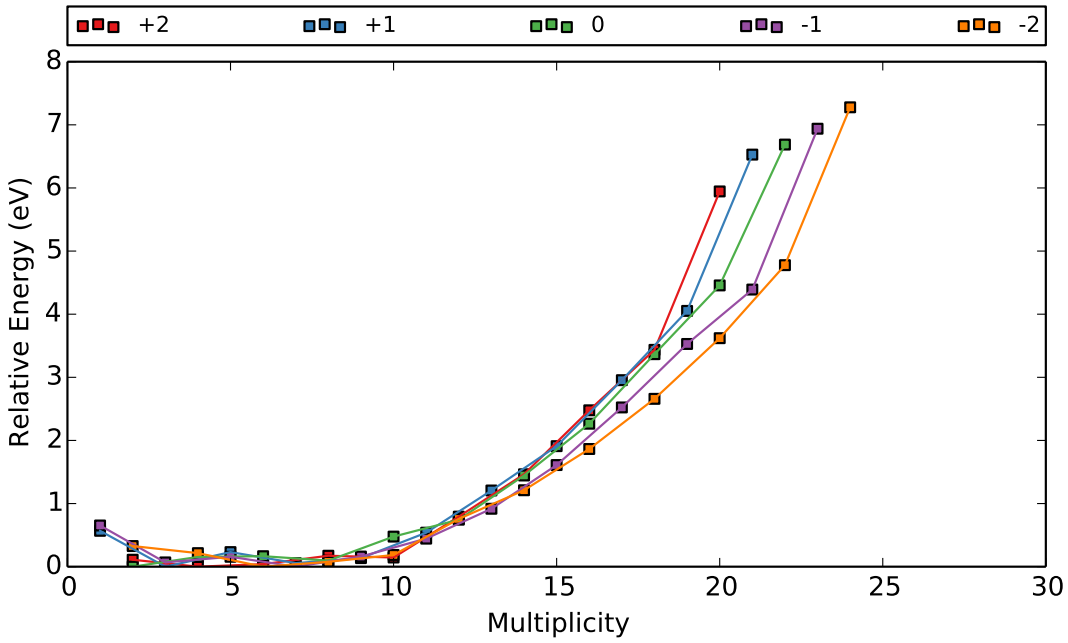

FIG. 14. Relative energies for the Yttrium cluster calculations for the PBE0 functional at each multiplicity. The energies are all relative to the lowest energy for each charge state i.e. the ground state energy is set to 0.

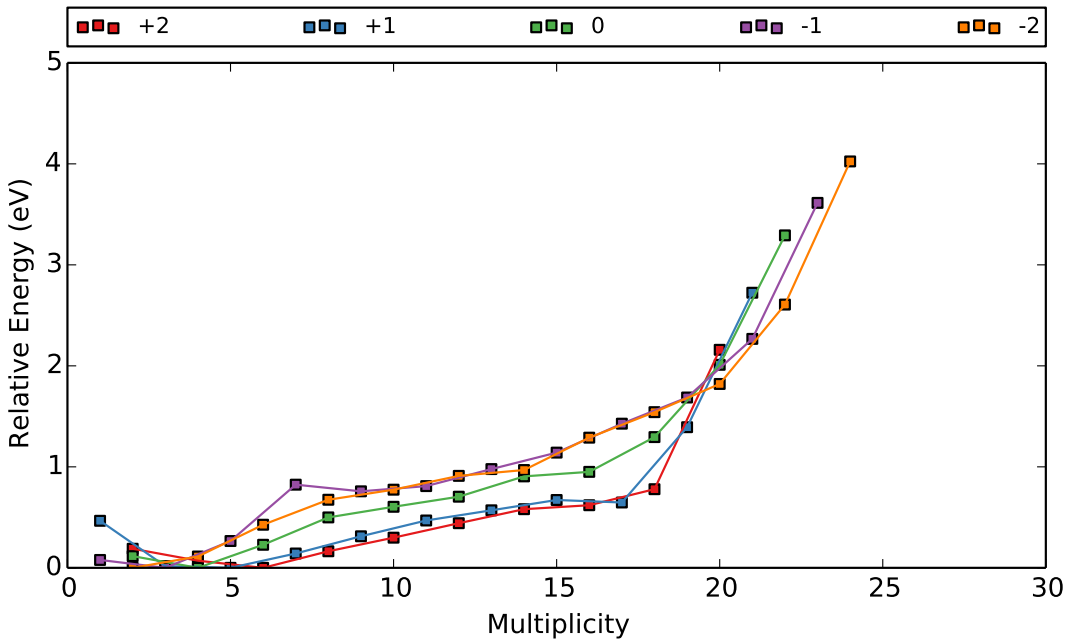

FIG. 15. Relative energies for the Lanthanum cluster calculations for the PBE0 functional at each multiplicity. The energies are all relative to the lowest energy for each charge state i.e. the ground state energy is set to 0.

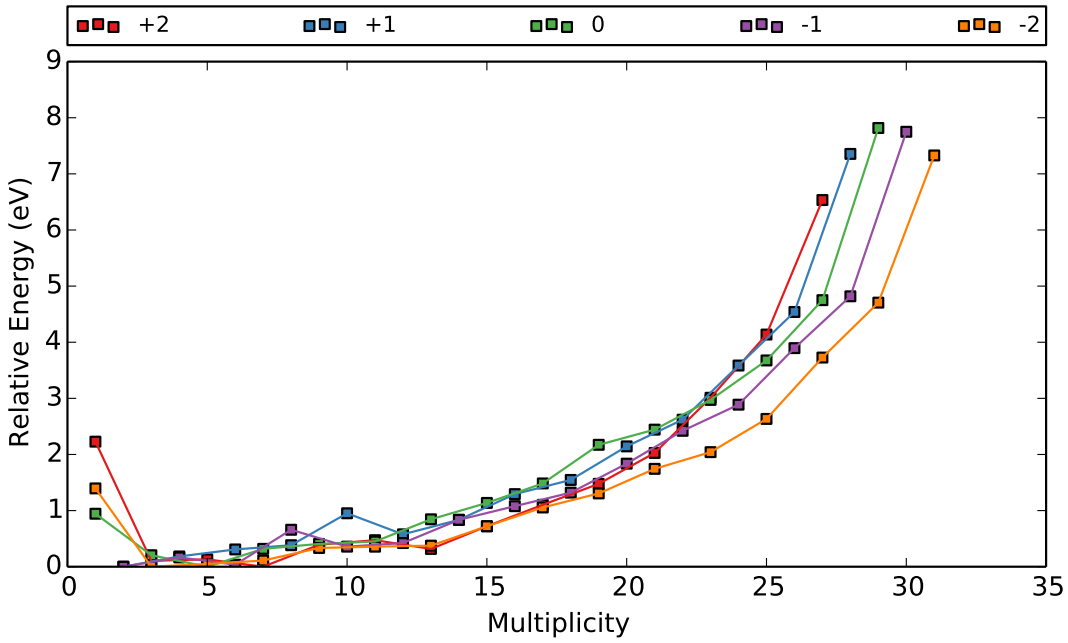

FIG. 16. Relative energies for the Titanium cluster calculations for the PBE0 functional at each multiplicity. The energies are all relative to the lowest energy for each charge state i.e. the ground state energy is set to 0.

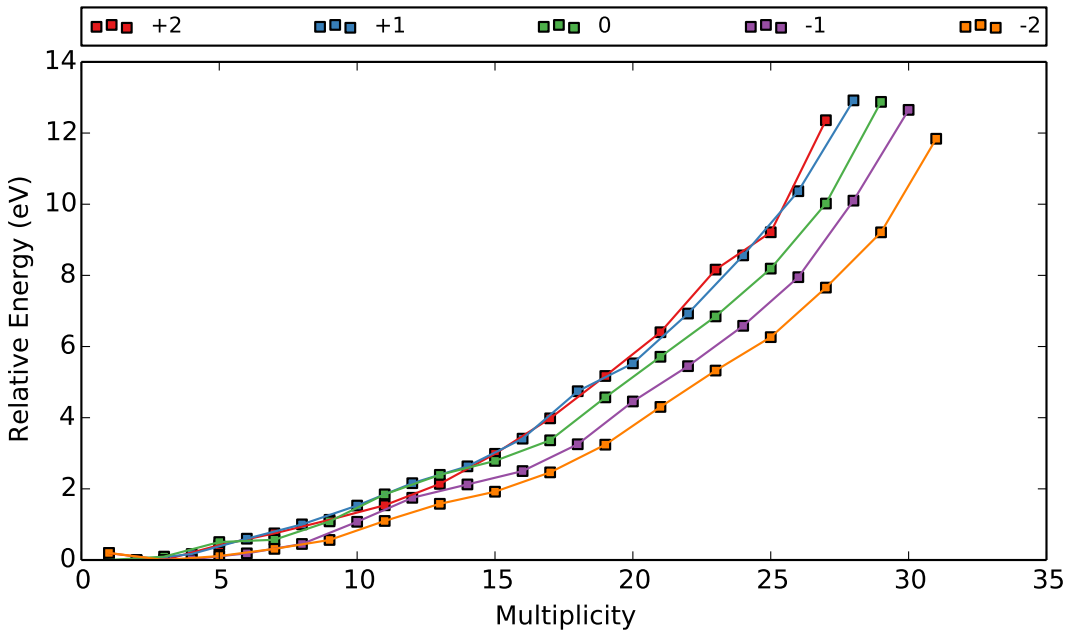

FIG. 17. Relative energies for the Zirconium cluster calculations for the PBE0 functional at each multiplicity. The energies are all relative to the lowest energy for each charge state i.e. the ground state energy is set to 0.

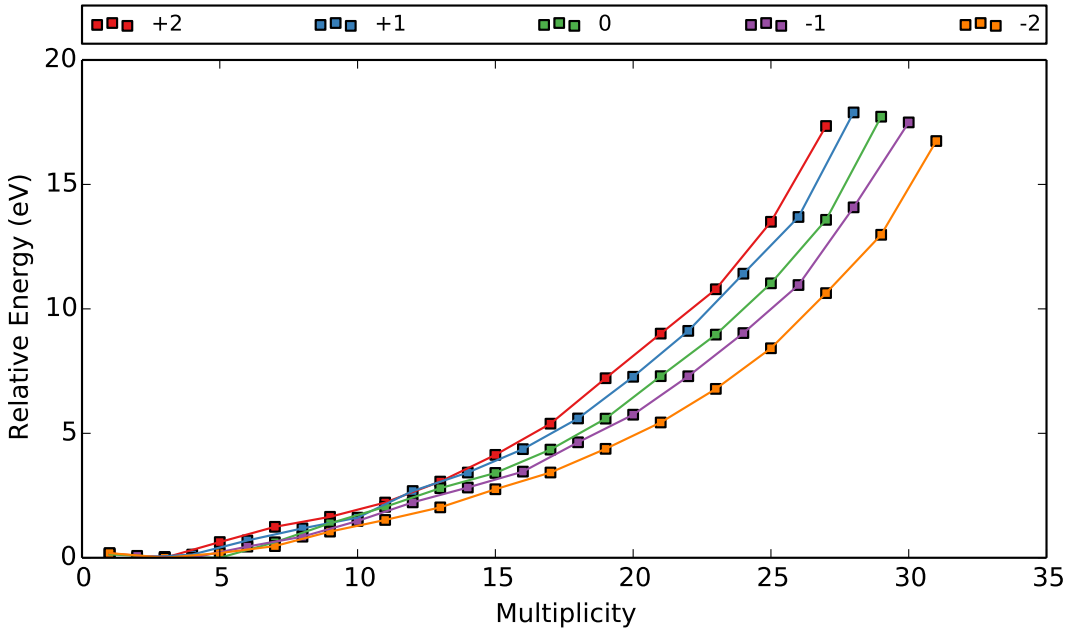

FIG. 18. Relative energies for the Hafnium cluster calculations for the PBE0 functional at each multiplicity. The energies are all relative to the lowest energy for each charge state i.e. the ground state energy is set to 0.