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

On the influence of exact exchange on transition metal superatoms - Supplementary Information

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I. PROJECTED DENSITY OF STATES

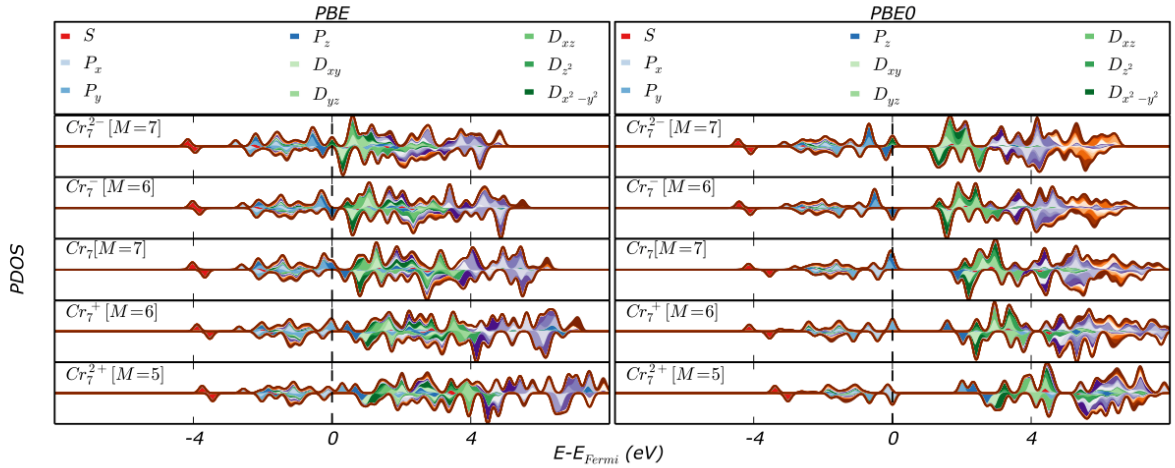

FIG. 1. Projected local density of states for the Cr_7^c (c = 0, ±1, ±2) cluster for the PBE and PBE0 exchange-correlation functionals. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts. Accompanying each plot is a label of the cluster charge, with the net multiplicity given in square brackets.

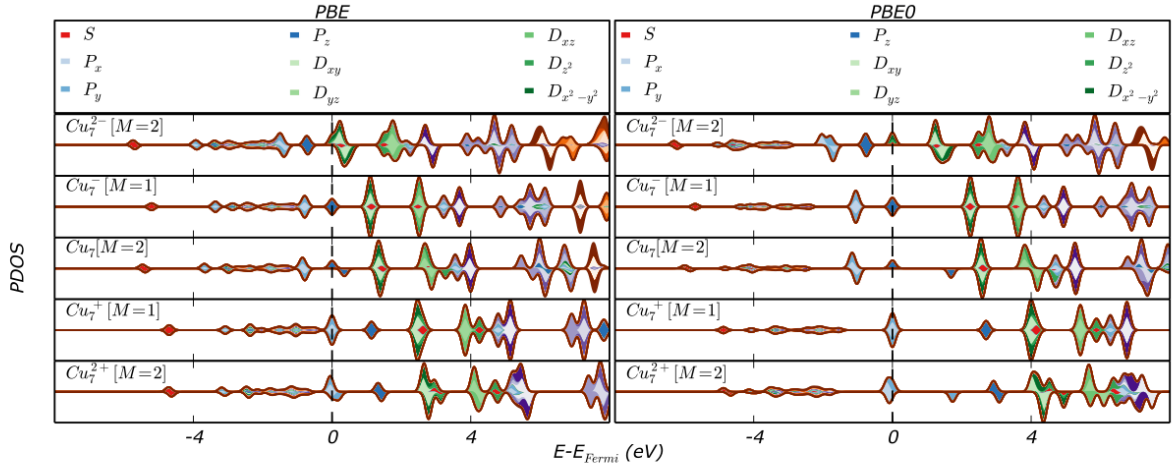

FIG. 2. Projected local density of states for the Cu_7^c (c = 0, ±1, ±2) cluster for the PBE and PBE0 exchange-correlation functionals. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts. Accompanying each plot is a label of the cluster charge, with the net multiplicity given in square brackets.

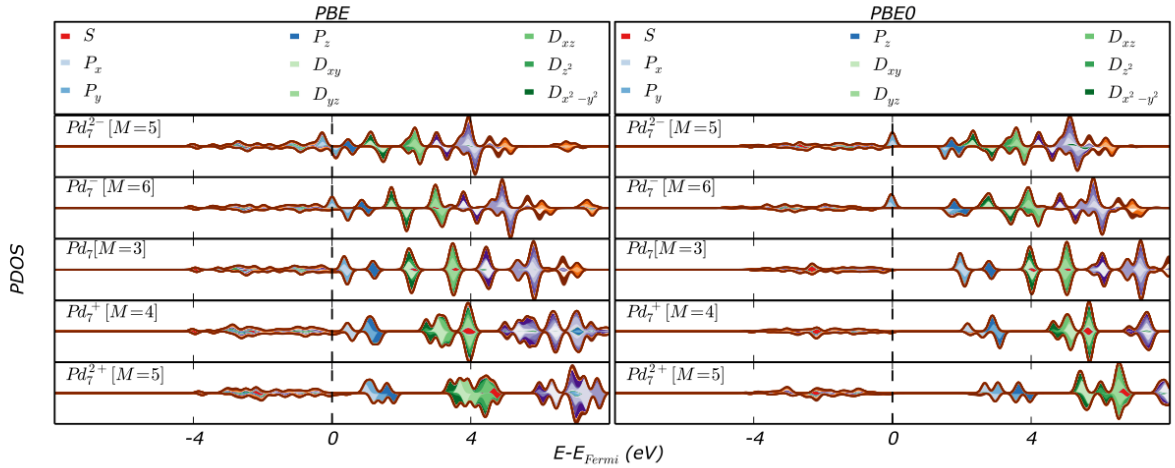

FIG. 3. Projected local density of states for the $Pd_7{}^c$ (c = 0, ±1, ±2) cluster for the PBE and PBE0 exchange-correlation functionals. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts. Accompanying each plot is a label of the cluster charge, with the net multiplicity given in square brackets.

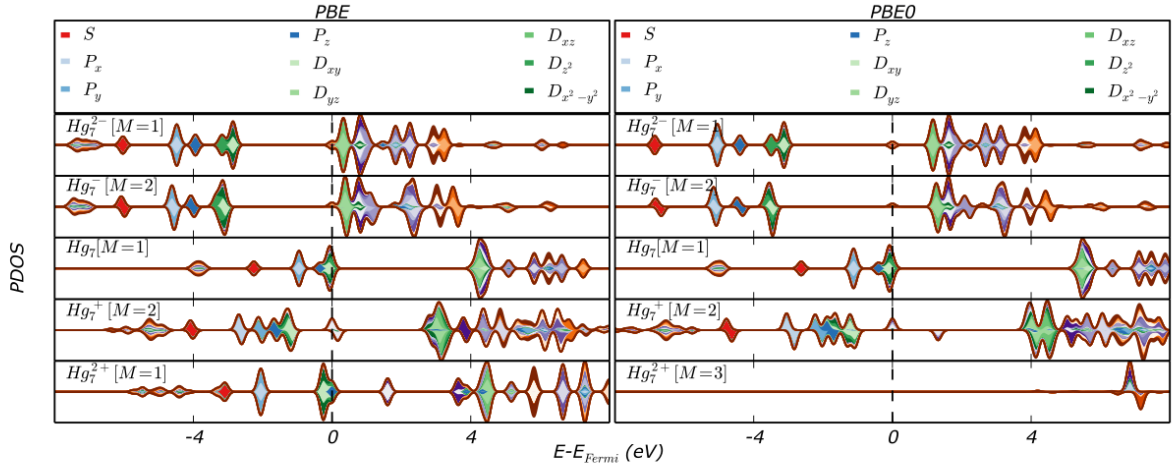

FIG. 4. Projected local density of states for the $Hg_7{}^c$ (c = 0, ±1, ±2) cluster for the PBE and PBE0 exchange-correlation functionals. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts. Accompanying each plot is a label of the cluster charge, with the net multiplicity given in square brackets.

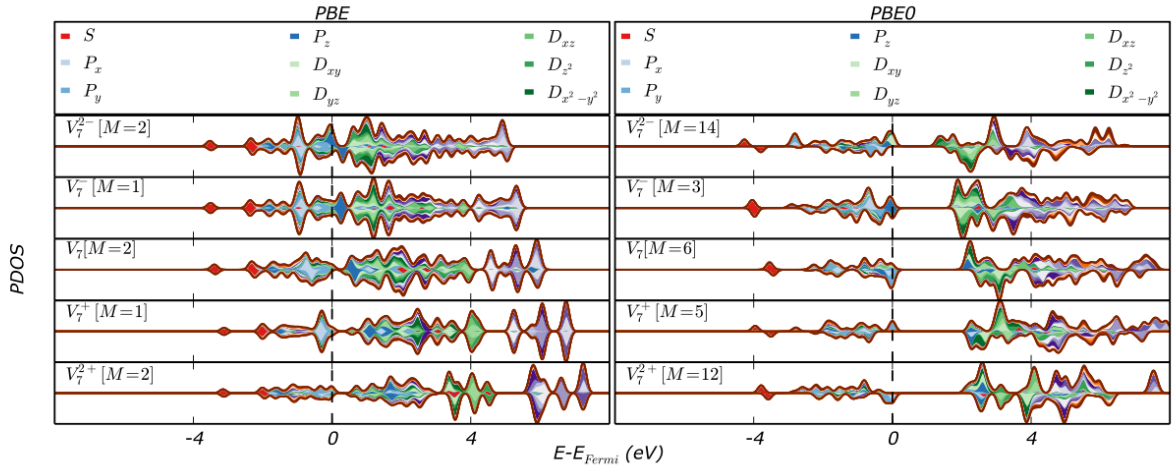

FIG. 5. Projected local density of states for the $V_7{}^c$ (c = 0, ±1, ±2) cluster for the PBE and PBE0 exchange-correlation functionals. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts. Accompanying each plot is a label of the cluster charge, with the net multiplicity given in square brackets.

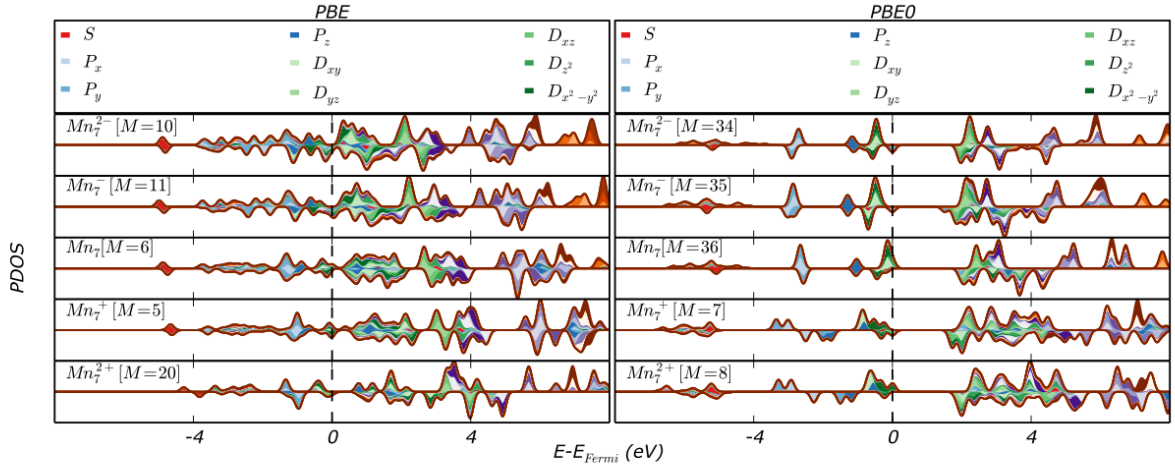

FIG. 6. Projected local density of states for the $Mn_7{}^c$ (c = 0, ±1, ±2) cluster for the PBE and PBE0 exchange-correlation functionals. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts. Accompanying each plot is a label of the cluster charge, with the net multiplicity given in square brackets.

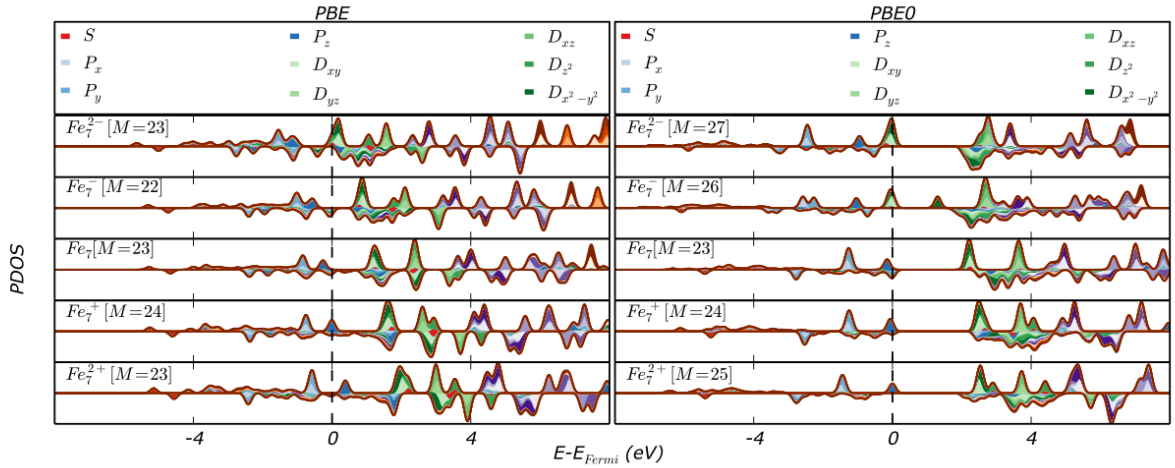

FIG. 7. Projected local density of states for the $Fe_7{}^c$ (c = 0, ±1, ±2) cluster for the PBE and PBE0 exchange-correlation functionals. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts. Accompanying each plot is a label of the cluster charge, with the net multiplicity given in square brackets.

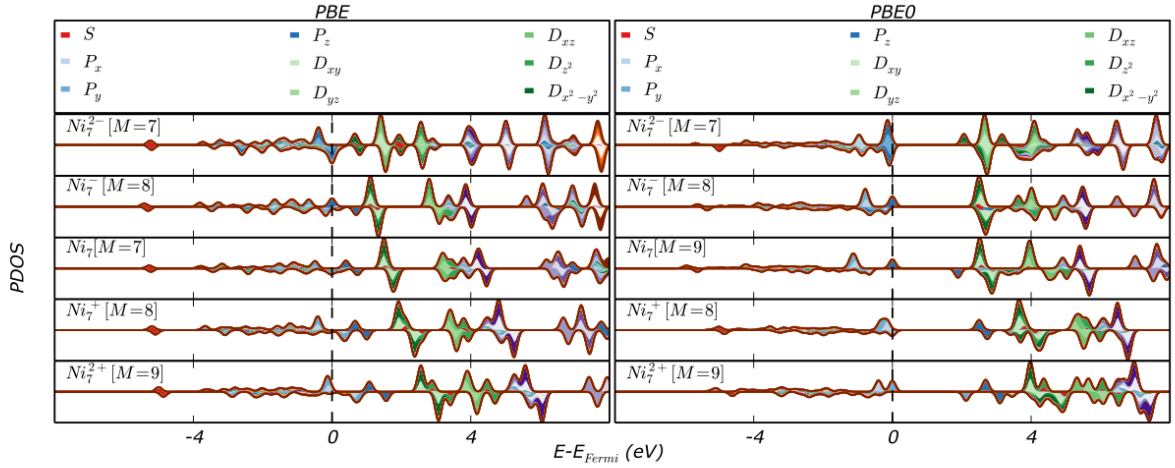

FIG. 8. Projected local density of states for the $Ni_7{}^c$ (c = 0, ±1, ±2) cluster for the PBE and PBE0 exchange-correlation functionals. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts. Accompanying each plot is a label of the cluster charge, with the net multiplicity given in square brackets.

II. PBE PROJECTED LOCAL DENSITY OF STATES

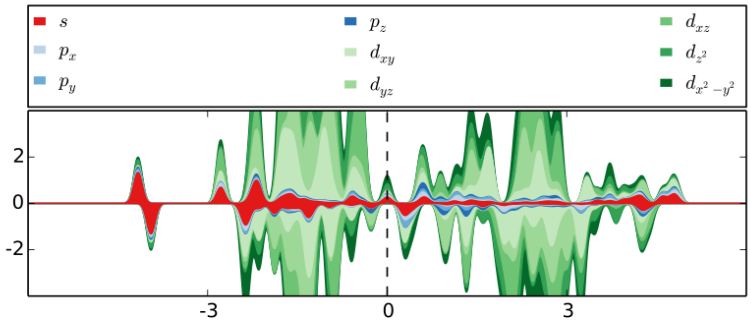

FIG. 9. Projected local density of states for the $Cr_7{}^{2-}$ cluster with a multiplicity of 7 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

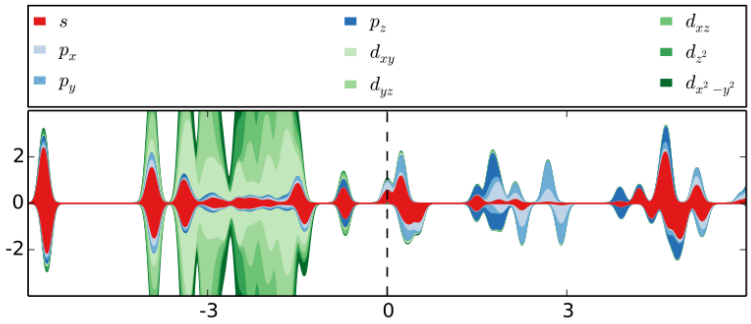

FIG. 10. Projected local density of states for the $Cu_7{}^{2-}$ cluster with a multiplicity of 2 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

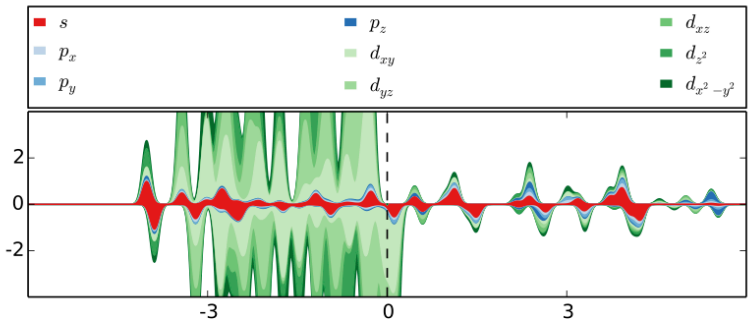

FIG. 11. Projected local density of states for the $Pd_7{}^{2-}$ cluster with a multiplicity of 5 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

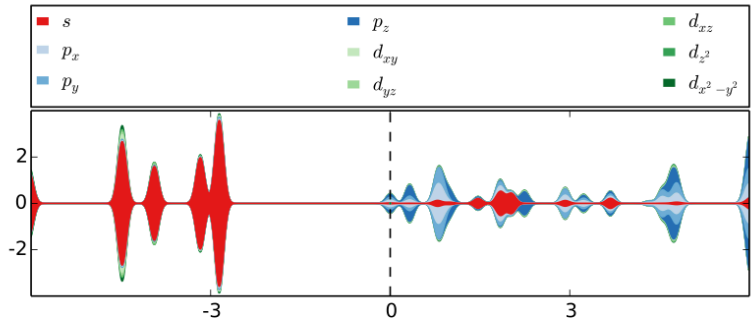

FIG. 12. Projected local density of states for the $Hg_7{}^{2-}$ cluster with a multiplicity of 1 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

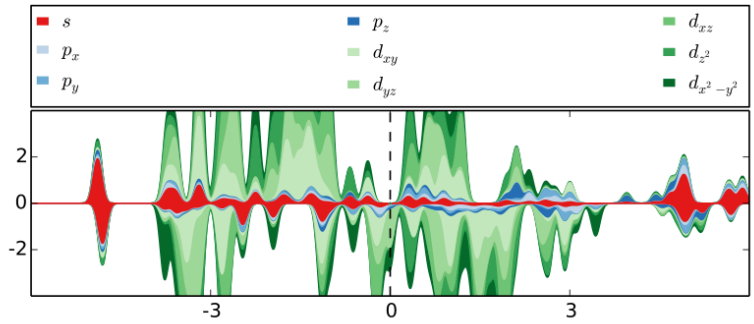

FIG. 13. Projected local density of states for the $Mn_7{}^{2-}$ cluster with a multiplicity of 10 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

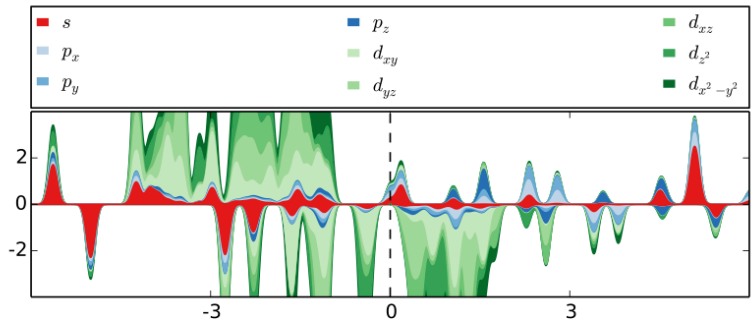

FIG. 14. Projected local density of states for the $Fe_7{}^{2-}$ cluster with a multiplicity of 23 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

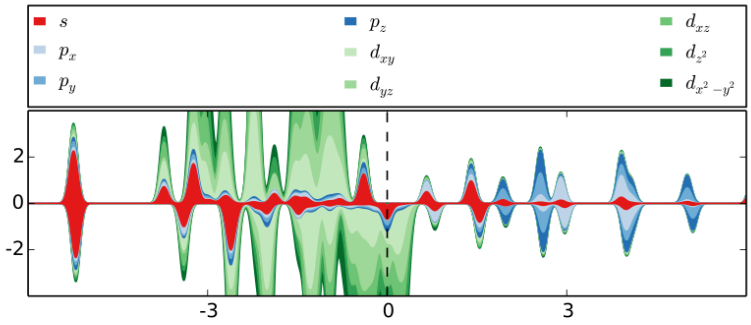

FIG. 15. Projected local density of states for the $Ni_7{}^{2-}$ cluster with a multiplicity of 7 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

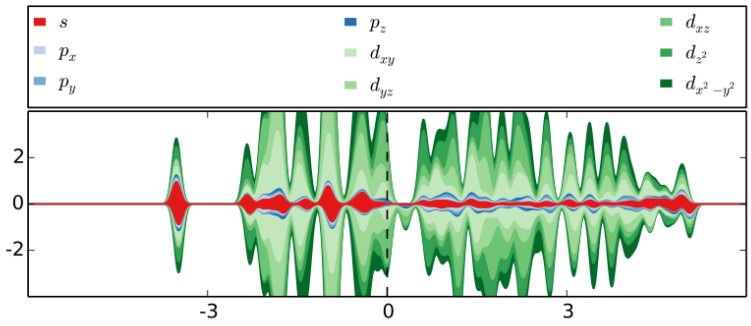

FIG. 16. Projected local density of states for the $V_7{}^{2-}$ cluster with a multiplicity of 2 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

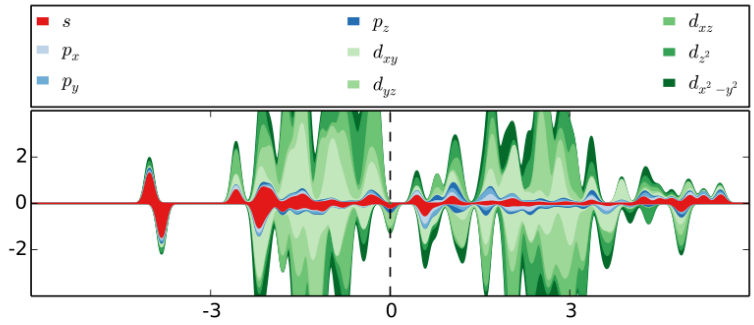

FIG. 17. Projected local density of states for the Cr_7^- cluster with a multiplicity of 6 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

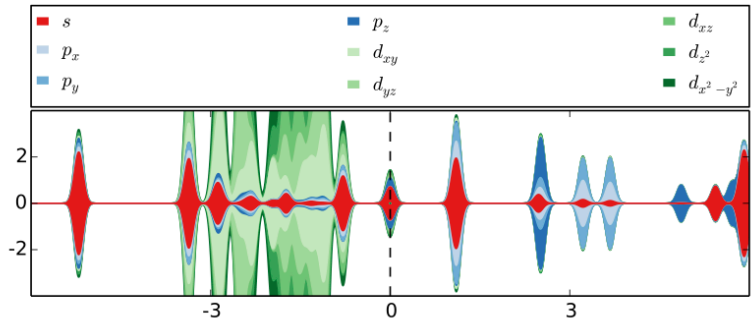

FIG. 18. Projected local density of states for the Cu_7^- cluster with a multiplicity of 1 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

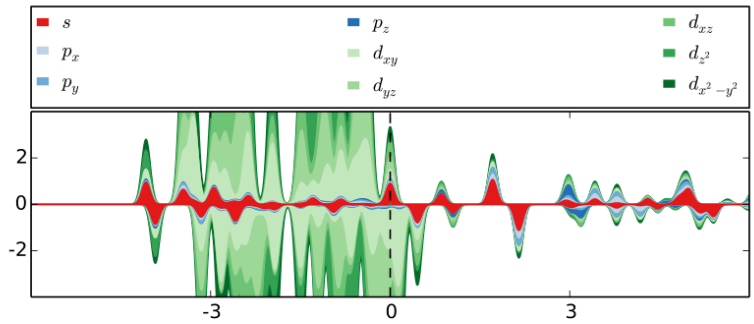

FIG. 19. Projected local density of states for the Pd_7^- cluster with a multiplicity of 6 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

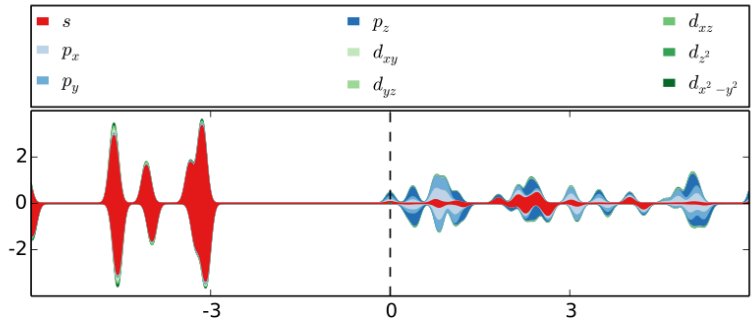

FIG. 20. Projected local density of states for the Hg_7^- cluster with a multiplicity of 2 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

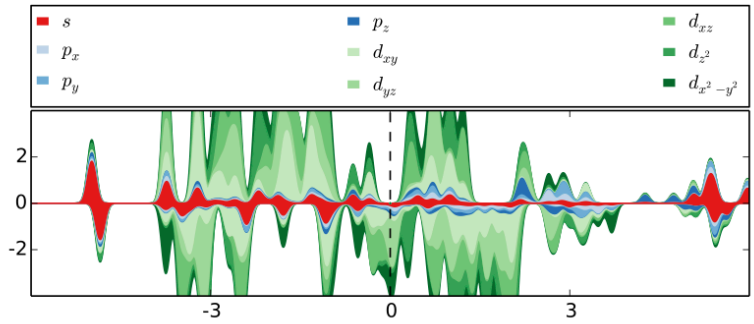

FIG. 21. Projected local density of states for the Mn_7^- cluster with a multiplicity of 11 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

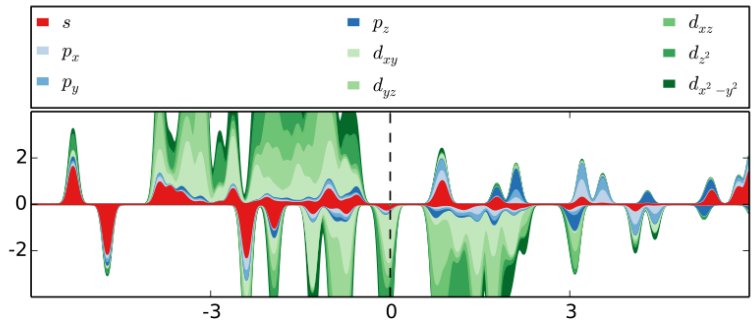

FIG. 22. Projected local density of states for the Fe_7^- cluster with a multiplicity of 22 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

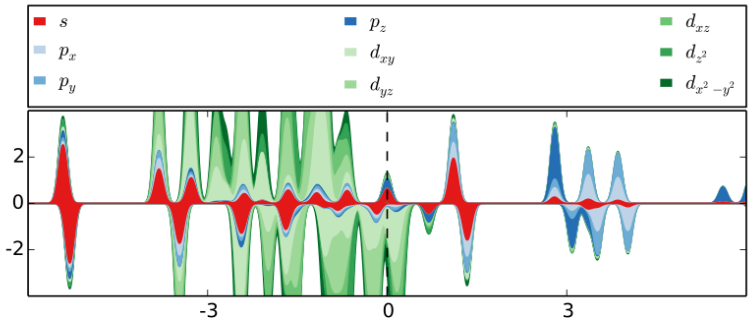

FIG. 23. Projected local density of states for the Ni_7^- cluster with a multiplicity of 8 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

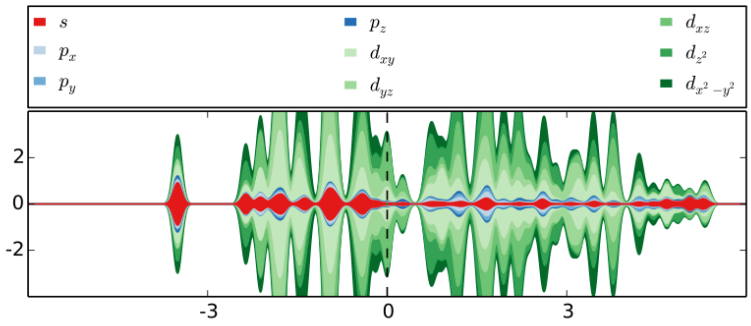

FIG. 24. Projected local density of states for the V_7^- cluster with a multiplicity of 1 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

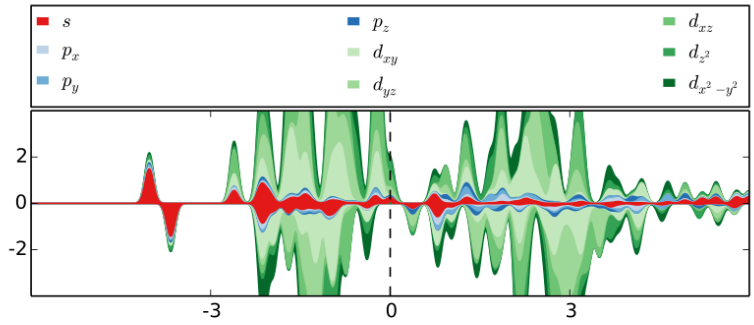

FIG. 25. Projected local density of states for the Cr_7 cluster with a multiplicity of 7 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

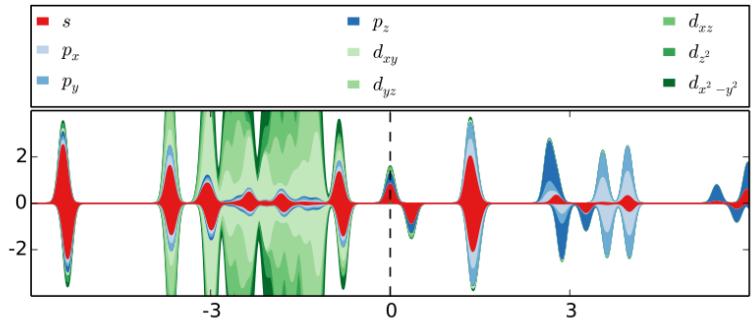

FIG. 26. Projected local density of states for the Cu_7 cluster with a multiplicity of 2 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

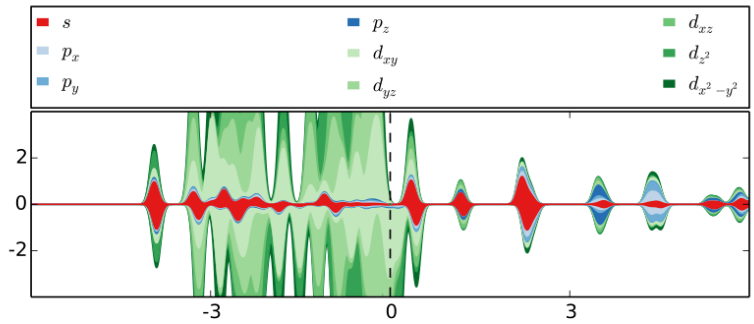

FIG. 27. Projected local density of states for the Pd_7 cluster with a multiplicity of 3 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

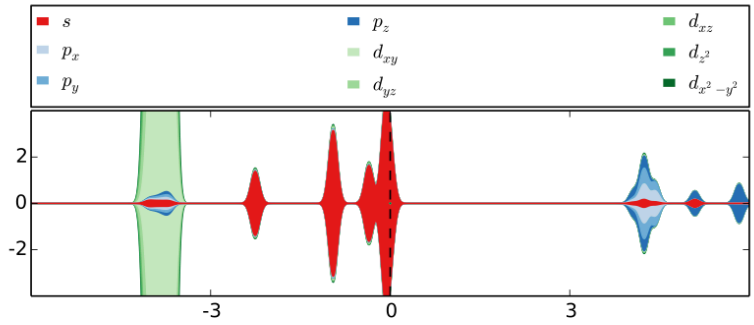

FIG. 28. Projected local density of states for the Hg_7 cluster with a multiplicity of 1 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

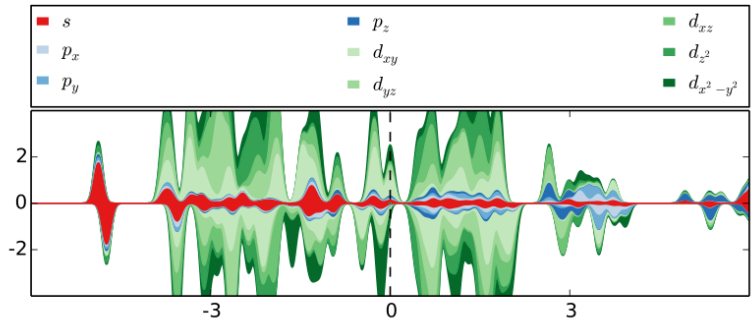

FIG. 29. Projected local density of states for the Mn_7 cluster with a multiplicity of 6 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

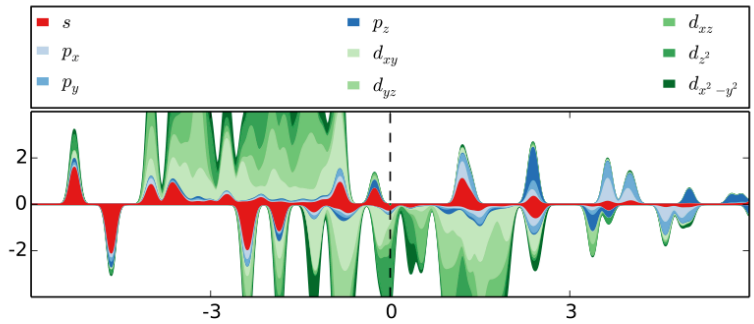

FIG. 30. Projected local density of states for the Fe_7 cluster with a multiplicity of 23 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

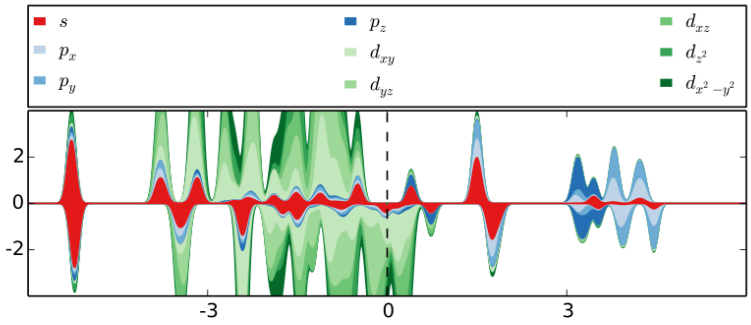

FIG. 31. Projected local density of states for the Ni_7 cluster with a multiplicity of 7 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

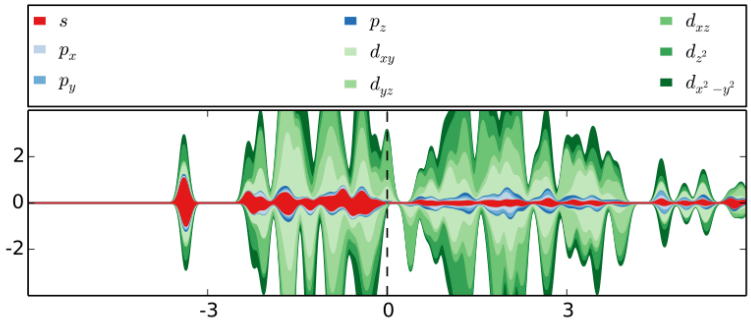

FIG. 32. Projected local density of states for the V_7 cluster with a multiplicity of 2 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

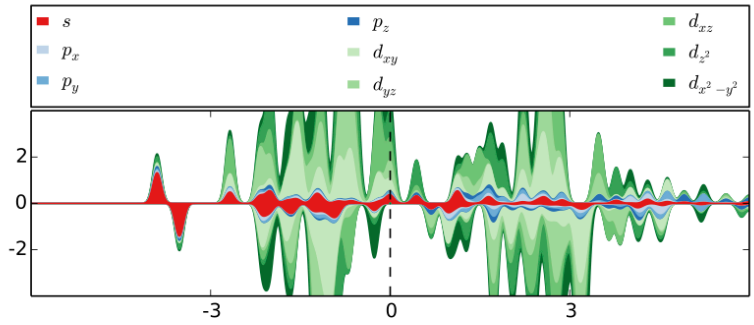

FIG. 33. Projected local density of states for the Cr_7^+ cluster with a multiplicity of 6 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

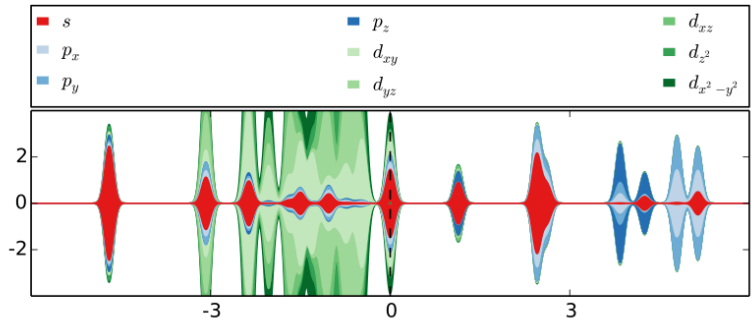

FIG. 34. Projected local density of states for the Cu_7^+ cluster with a multiplicity of 1 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

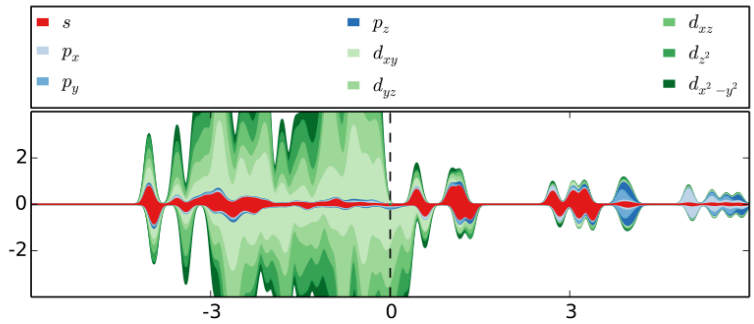

FIG. 35. Projected local density of states for the Pd_7^+ cluster with a multiplicity of 4 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

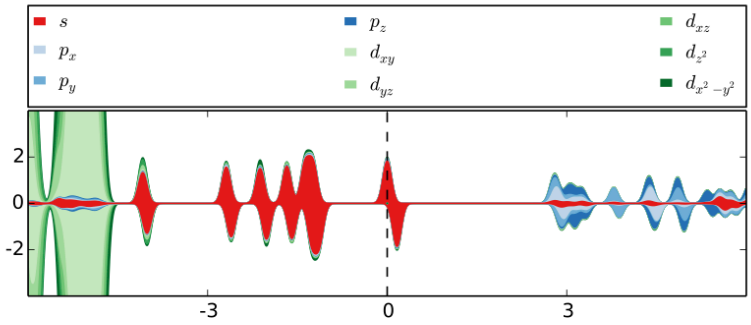

FIG. 36. Projected local density of states for the $Hg_7{}^+$ cluster with a multiplicity of 2 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

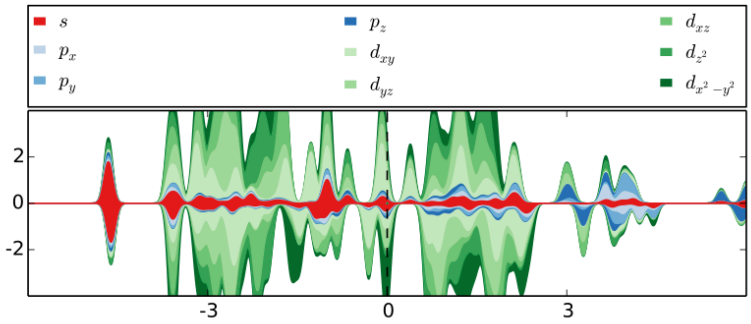

FIG. 37. Projected local density of states for the $Mn_7{}^+$ cluster with a multiplicity of 5 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

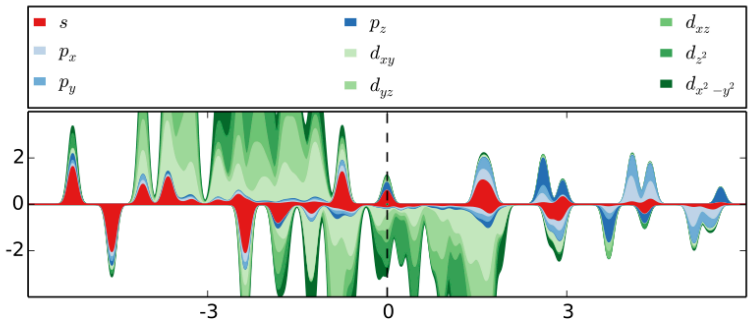

FIG. 38. Projected local density of states for the $Fe_7{}^+$ cluster with a multiplicity of 24 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

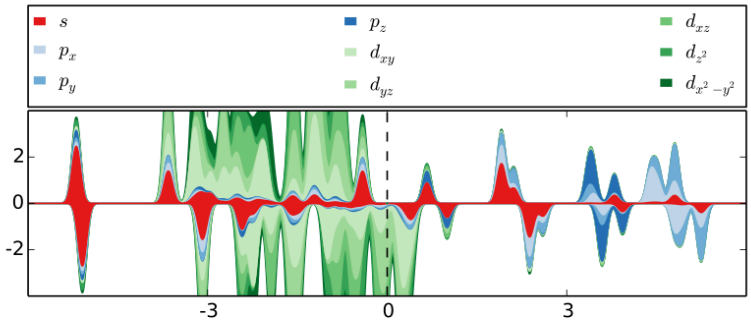

FIG. 39. Projected local density of states for the $Ni_7{}^+$ cluster with a multiplicity of 8 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

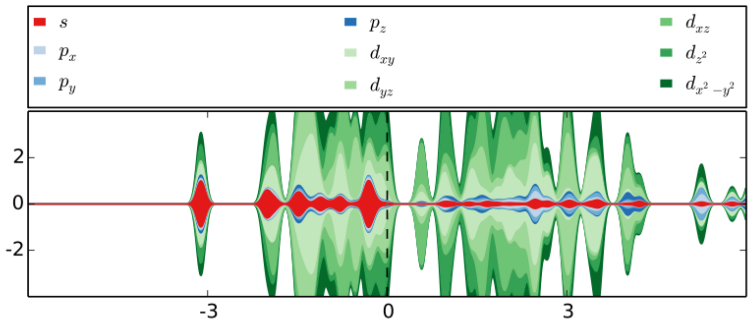

FIG. 40. Projected local density of states for the $V_7{}^+$ cluster with a multiplicity of 1 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

III. PBE0 PROJECTED LOCAL DENSITY OF STATES

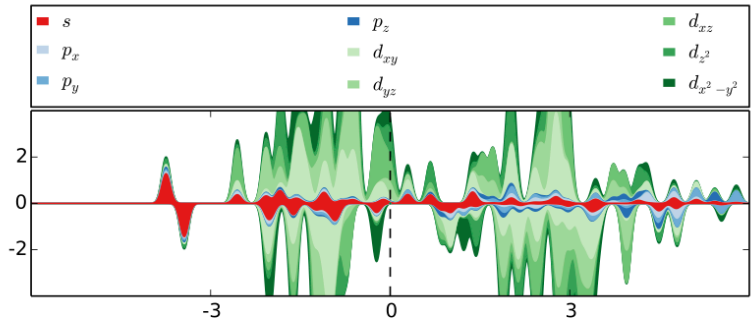

FIG. 41. Projected local density of states for the $Cr_7{}^{2+}$ cluster with a multiplicity of 5 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

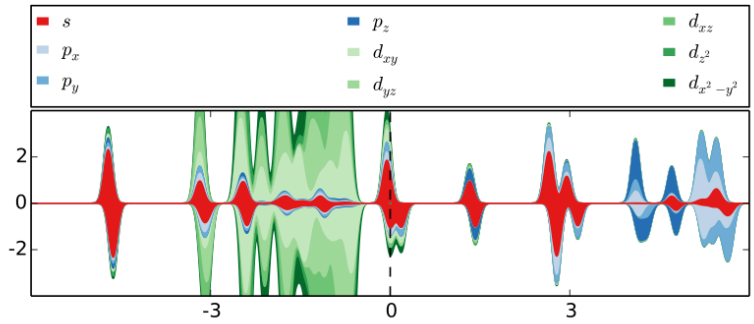

FIG. 42. Projected local density of states for the $Cu_7{}^{2+}$ cluster with a multiplicity of 2 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

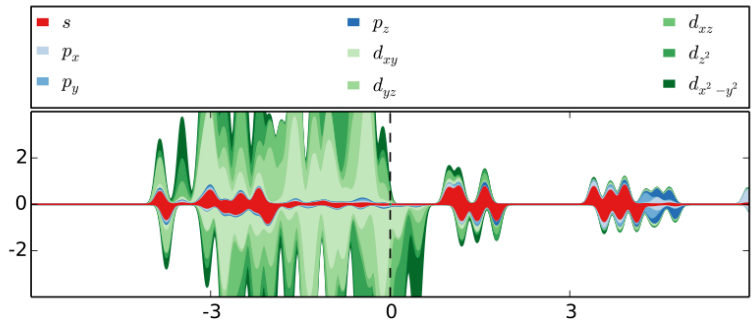

FIG. 43. Projected local density of states for the $Pd_7{}^{2+}$ cluster with a multiplicity of 5 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

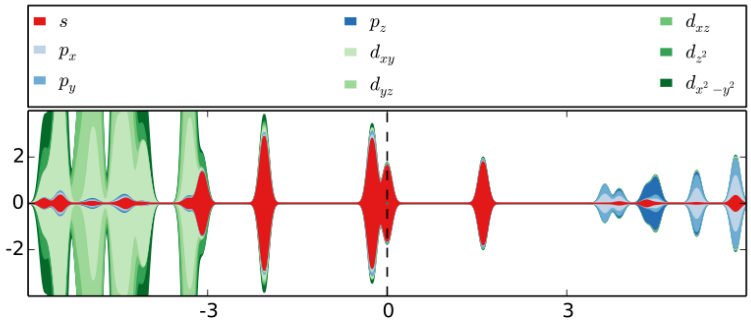

FIG. 44. Projected local density of states for the $Hg_7{}^{2+}$ cluster with a multiplicity of 1 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

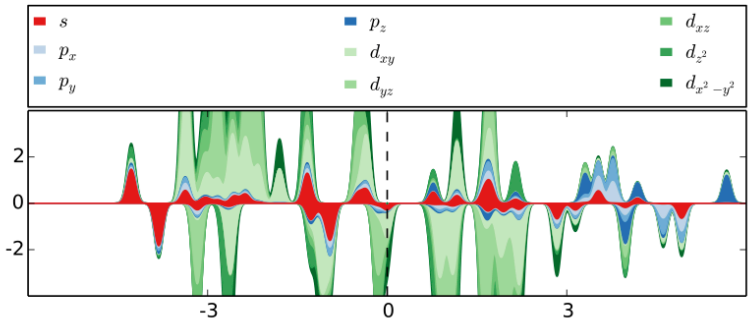

FIG. 45. Projected local density of states for the $Mn_7{}^{2+}$ cluster with a multiplicity of 20 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

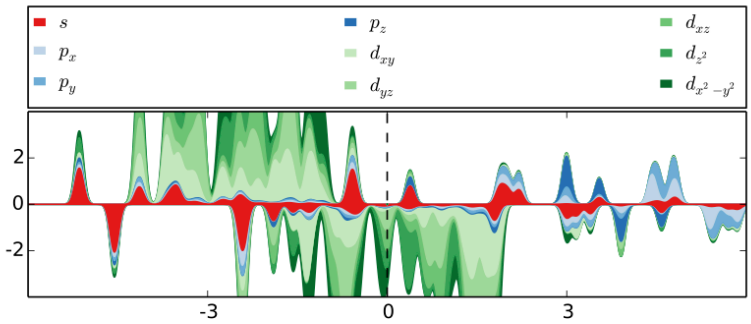

FIG. 46. Projected local density of states for the $Fe_7{}^{2+}$ cluster with a multiplicity of 23 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

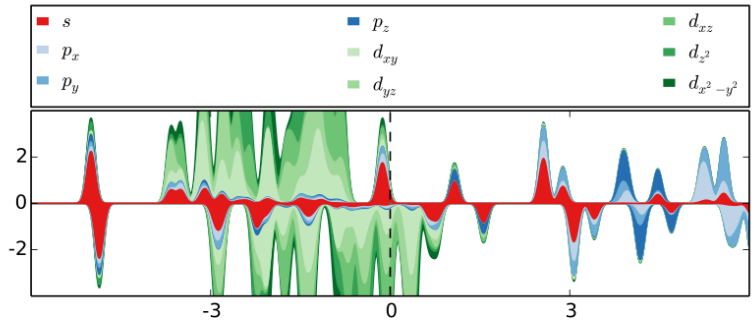

FIG. 47. Projected local density of states for the $Ni_7{}^{2+}$ cluster with a multiplicity of 9 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

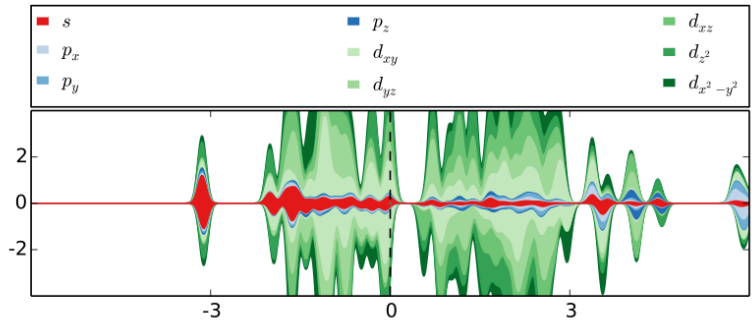

FIG. 48. Projected local density of states for the $V_7{}^{2+}$ cluster with a multiplicity of 2 for the PBE exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

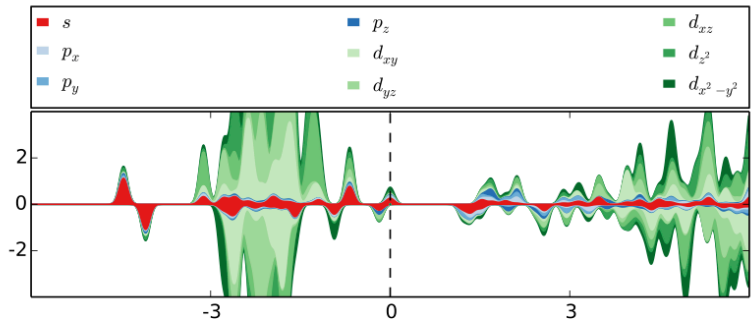

FIG. 49. Projected local density of states for the $Cr_7{}^{2-}$ cluster with a multiplicity of 7 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

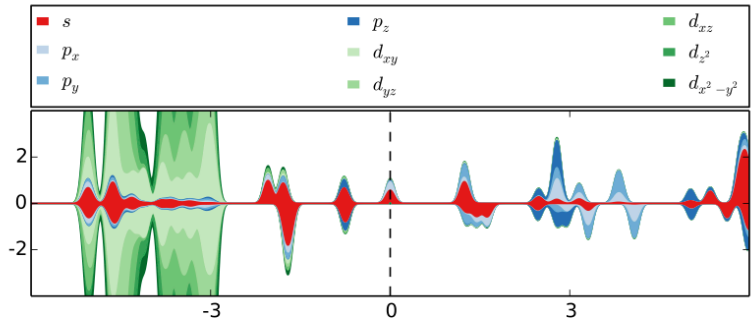

FIG. 50. Projected local density of states for the $Cu_7{}^{2-}$ cluster with a multiplicity of 2 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

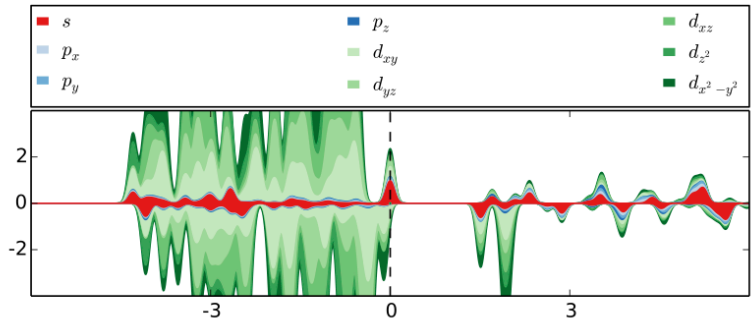

FIG. 51. Projected local density of states for the $Pd_7{}^{2-}$ cluster with a multiplicity of 5 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

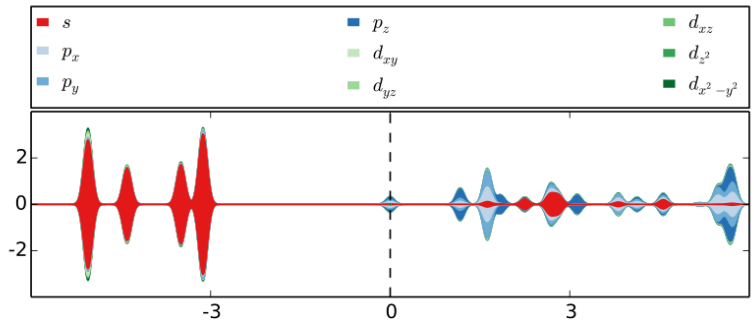

FIG. 52. Projected local density of states for the $Hg_7{}^{2-}$ cluster with a multiplicity of 1 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

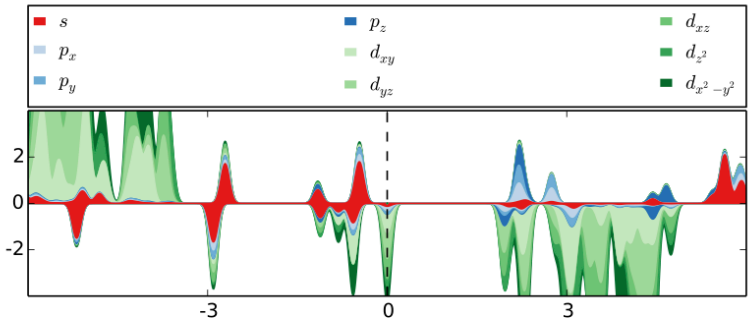

FIG. 53. Projected local density of states for the $Mn_7{}^{2-}$ cluster with a multiplicity of 34 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

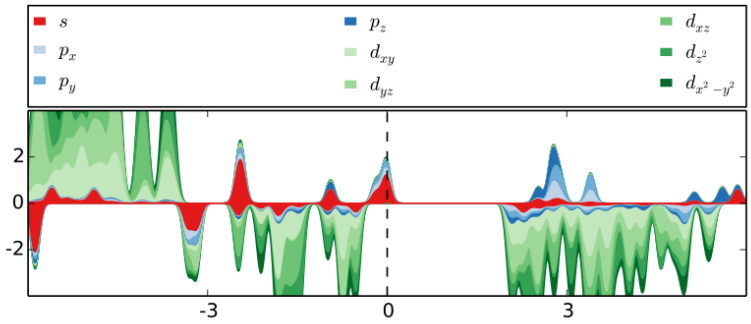

FIG. 54. Projected local density of states for the $Fe_7{}^{2-}$ cluster with a multiplicity of 27 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

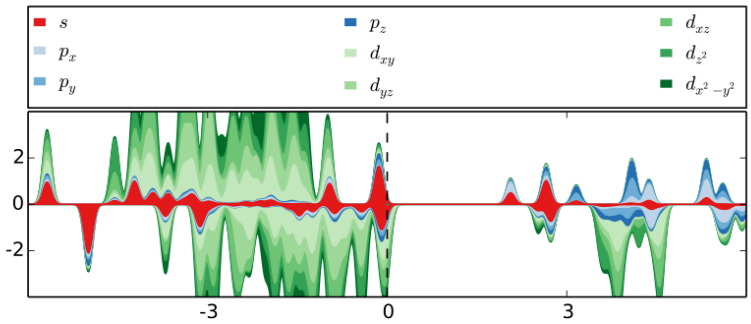

FIG. 55. Projected local density of states for the $Ni_7{}^{2-}$ cluster with a multiplicity of 7 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

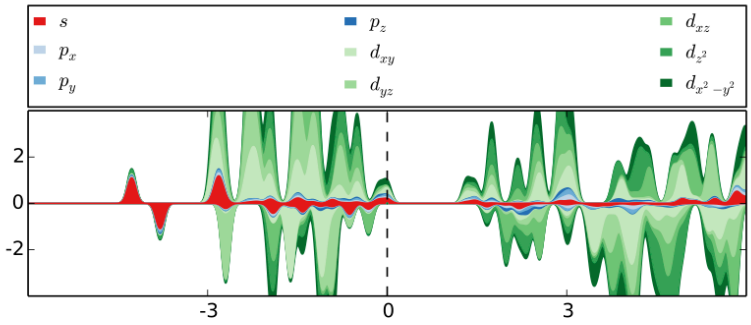

FIG. 56. Projected local density of states for the $V_7{}^{2-}$ cluster with a multiplicity of 14 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

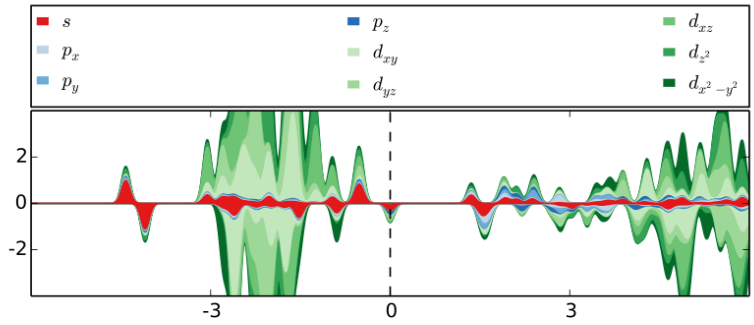

FIG. 57. Projected local density of states for the Cr_7^- cluster with a multiplicity of 6 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

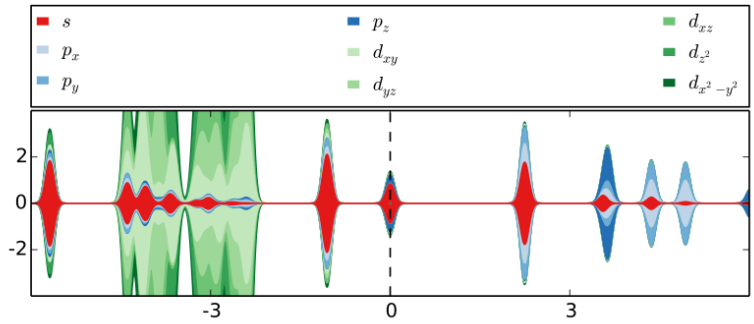

FIG. 58. Projected local density of states for the Cu_7^- cluster with a multiplicity of 1 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

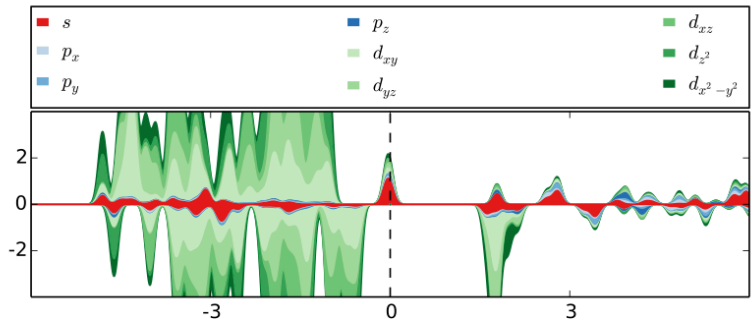

FIG. 59. Projected local density of states for the Pd_7^- cluster with a multiplicity of 6 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

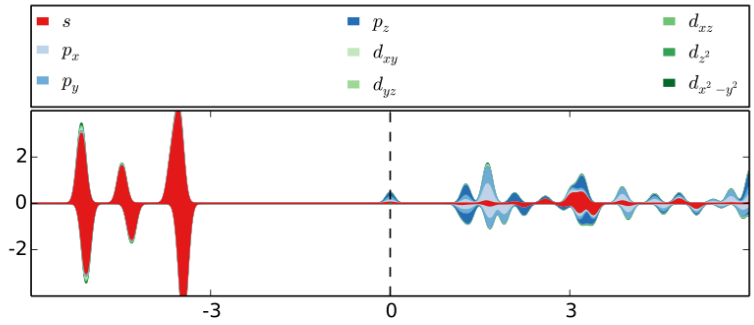

FIG. 60. Projected local density of states for the Hg_7^- cluster with a multiplicity of 2 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

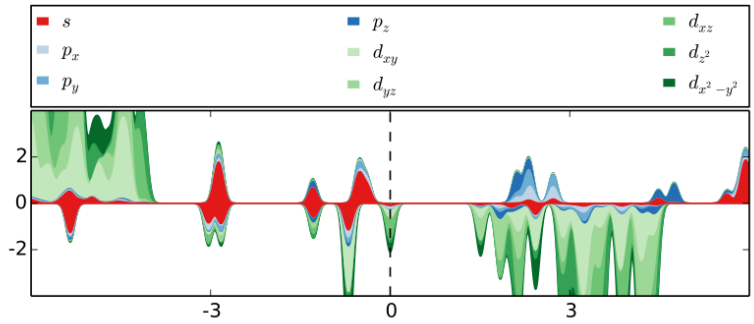

FIG. 61. Projected local density of states for the Mn_7^- cluster with a multiplicity of 35 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

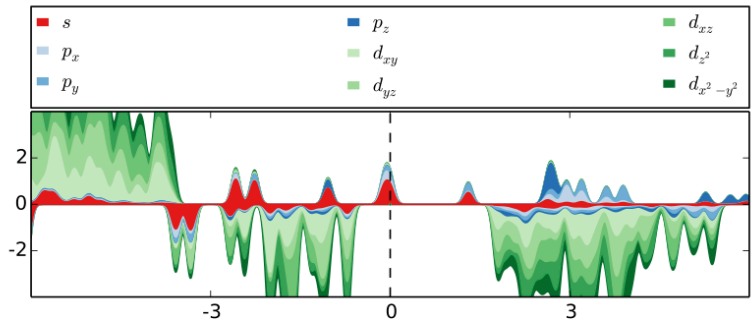

FIG. 62. Projected local density of states for the Fe_7^- cluster with a multiplicity of 26 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

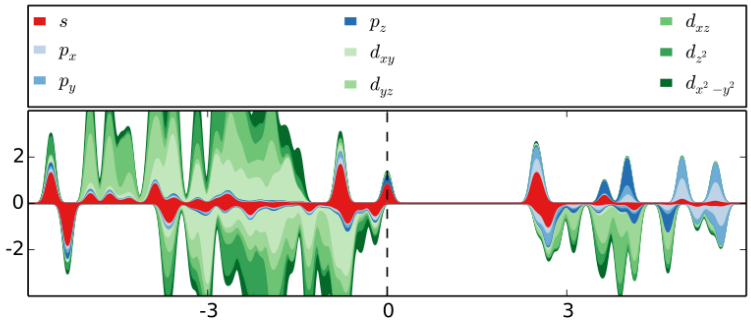

FIG. 63. Projected local density of states for the Ni_7^- cluster with a multiplicity of 8 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

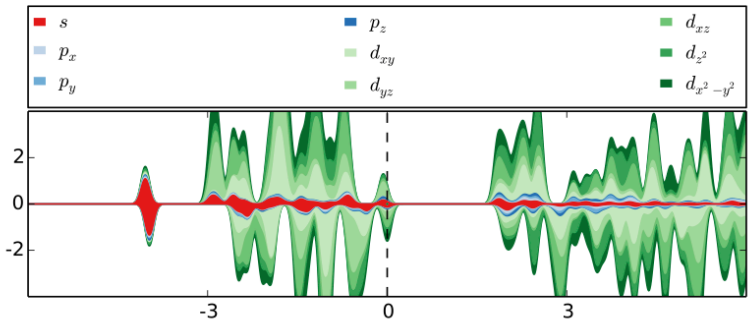

FIG. 64. Projected local density of states for the V_7^- cluster with a multiplicity of 3 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

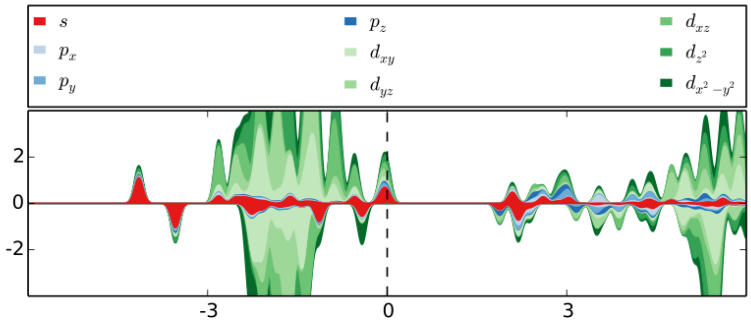

FIG. 65. Projected local density of states for the Cr_7 cluster with a multiplicity of 7 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

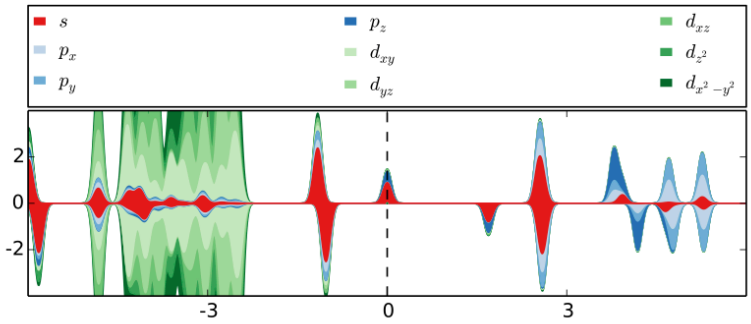

FIG. 66. Projected local density of states for the Cu_7 cluster with a multiplicity of 2 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

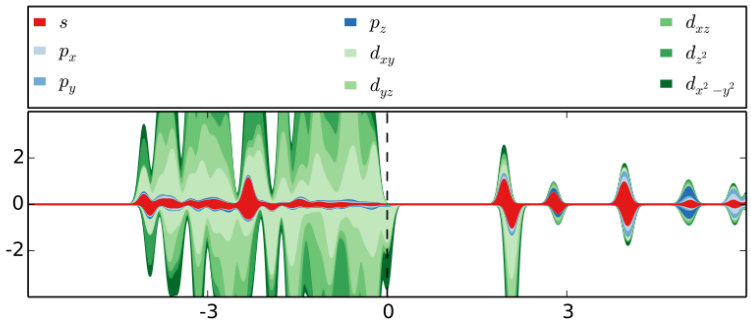

FIG. 67. Projected local density of states for the Pd_7 cluster with a multiplicity of 3 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

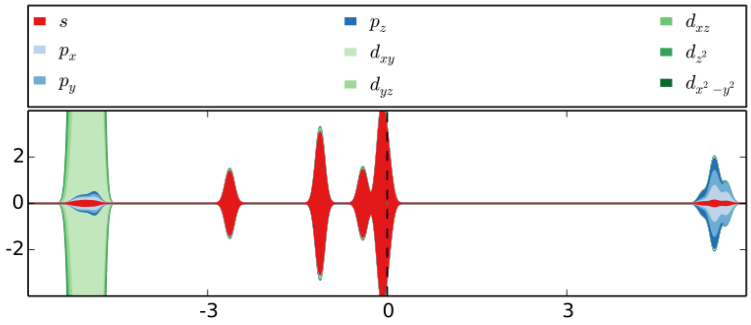

FIG. 68. Projected local density of states for the Hg_7 cluster with a multiplicity of 1 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

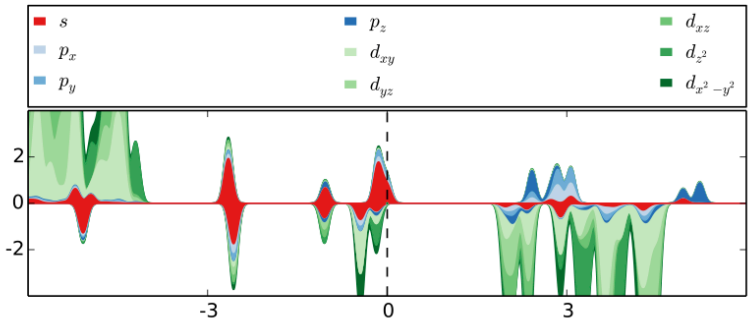

FIG. 69. Projected local density of states for the Mn_7 cluster with a multiplicity of 36 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

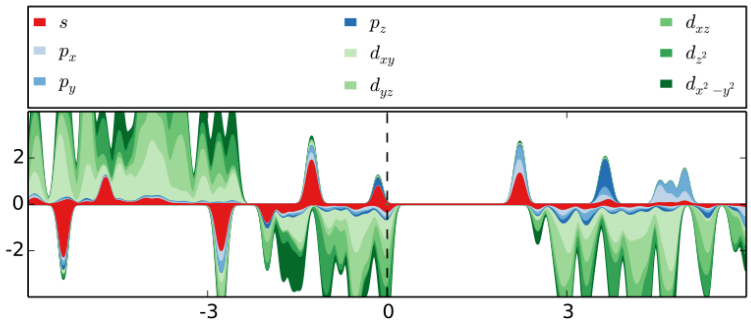

FIG. 70. Projected local density of states for the Fe_7 cluster with a multiplicity of 23 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

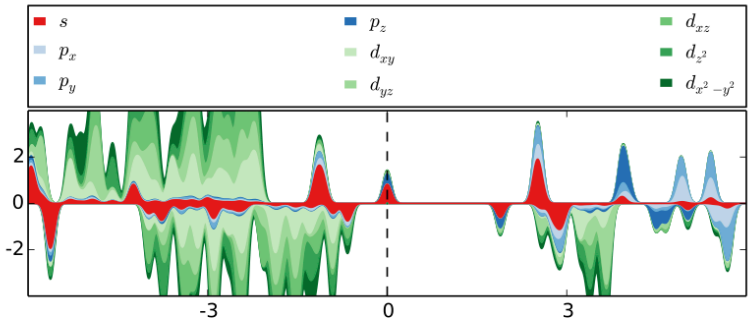

FIG. 71. Projected local density of states for the Ni_7 cluster with a multiplicity of 9 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

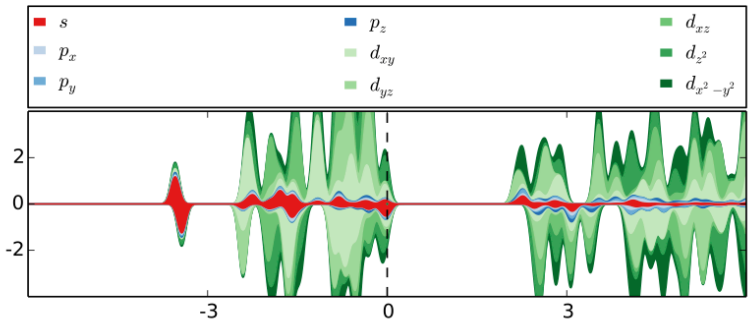

FIG. 72. Projected local density of states for the V_7 cluster with a multiplicity of 6 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

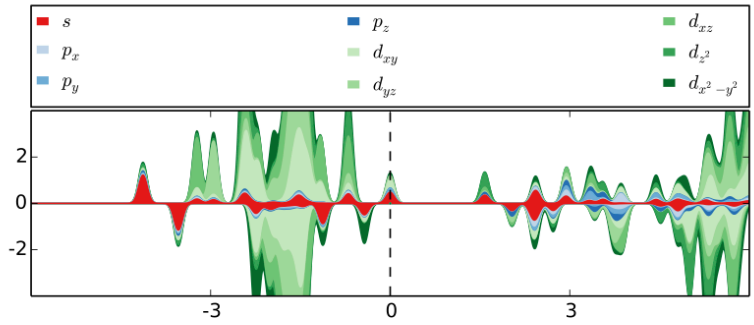

FIG. 73. Projected local density of states for the $Cr_7{}^+$ cluster with a multiplicity of 6 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

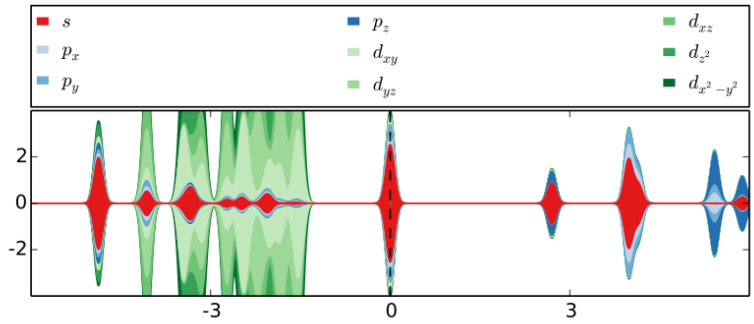

FIG. 74. Projected local density of states for the $Cu_7{}^+$ cluster with a multiplicity of 1 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

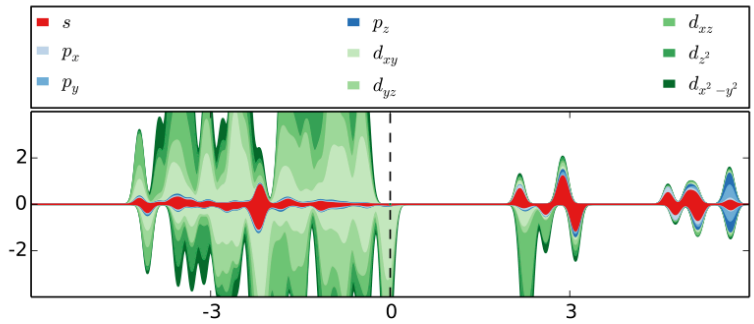

FIG. 75. Projected local density of states for the $Pd_7{}^+$ cluster with a multiplicity of 4 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

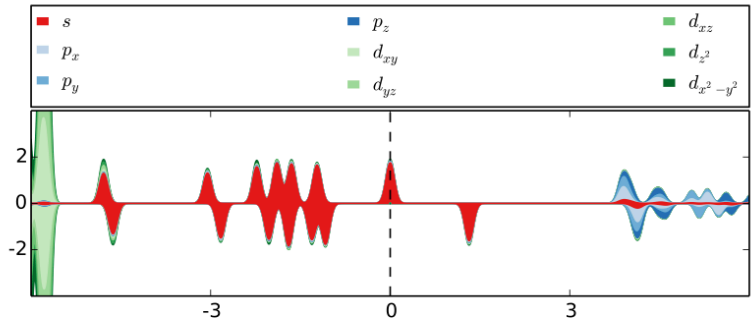

FIG. 76. Projected local density of states for the $Hg_7{}^+$ cluster with a multiplicity of 2 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

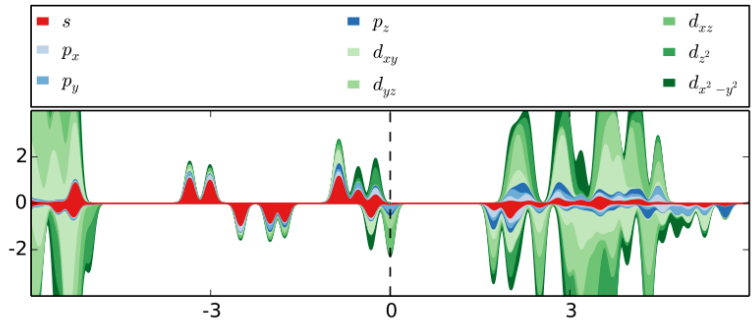

FIG. 77. Projected local density of states for the $Mn_7{}^+$ cluster with a multiplicity of 7 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

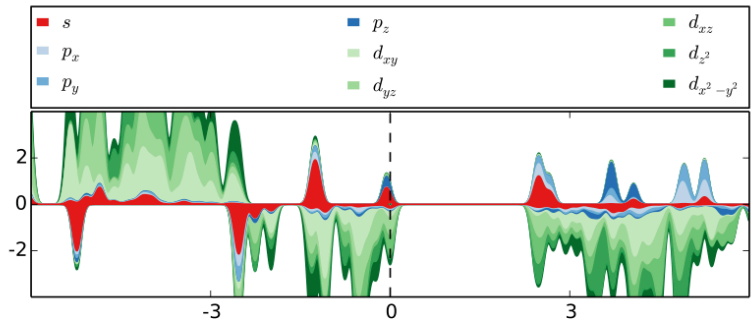

FIG. 78. Projected local density of states for the $Fe_7{}^+$ cluster with a multiplicity of 24 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

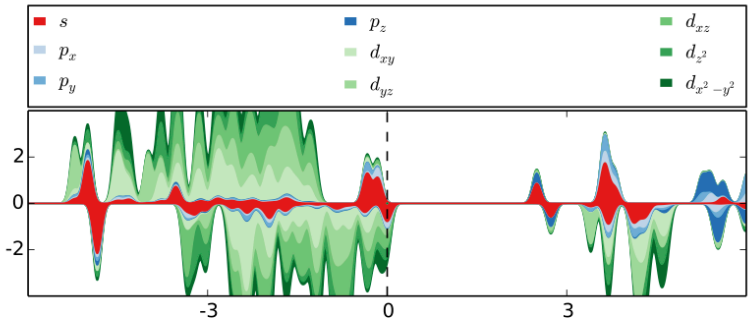

FIG. 79. Projected local density of states for the $Ni_7{}^+$ cluster with a multiplicity of 8 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

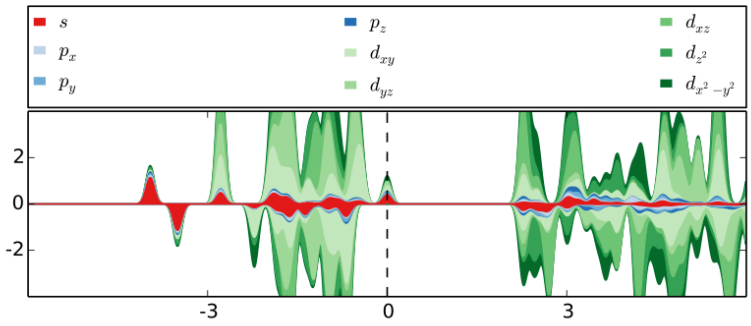

FIG. 80. Projected local density of states for the $V_7{}^+$ cluster with a multiplicity of 5 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

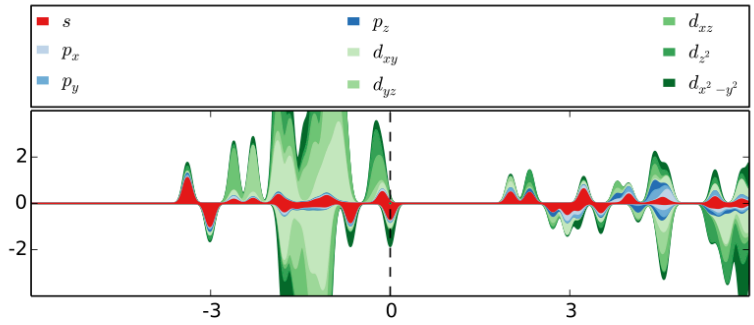

FIG. 81. Projected local density of states for the $Cr_7{}^{2+}$ cluster with a multiplicity of 5 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

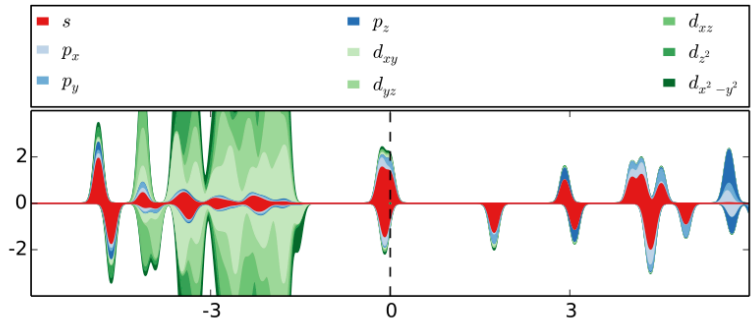

FIG. 82. Projected local density of states for the $Cu_7{}^{2+}$ cluster with a multiplicity of 2 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

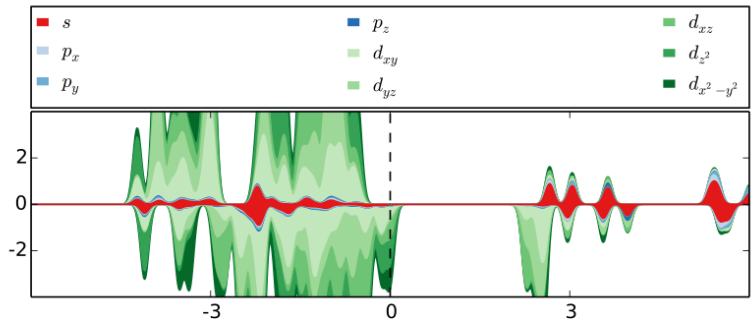

FIG. 83. Projected local density of states for the $Pd_7{}^{2+}$ cluster with a multiplicity of 5 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

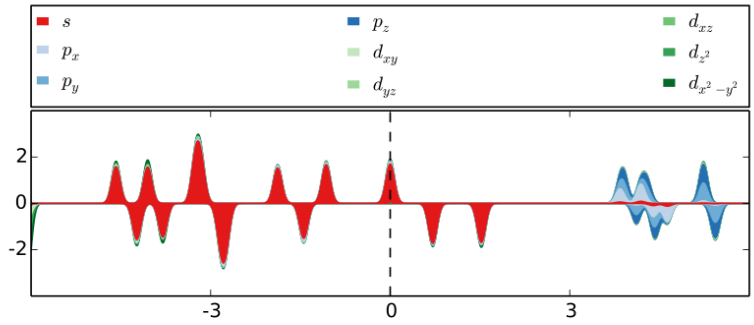

FIG. 84. Projected local density of states for the $Hg_7{}^{2+}$ cluster with a multiplicity of 3 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

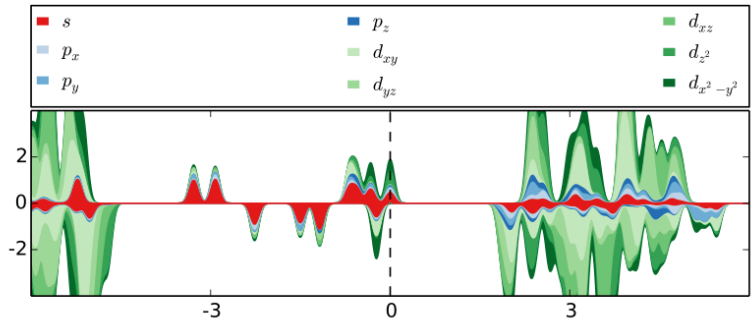

FIG. 85. Projected local density of states for the $Mn_7{}^{2+}$ cluster with a multiplicity of 8 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

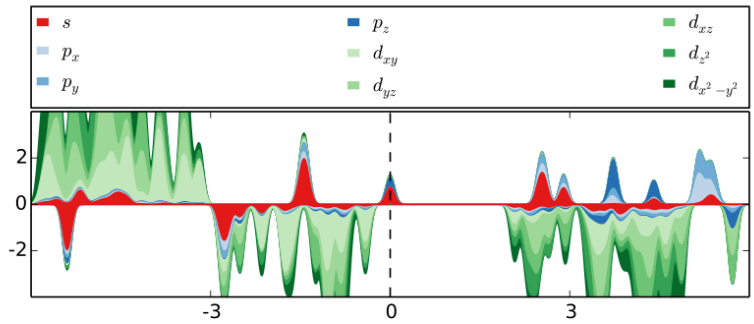

FIG. 86. Projected local density of states for the $Fe_7{}^{2+}$ cluster with a multiplicity of 25 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

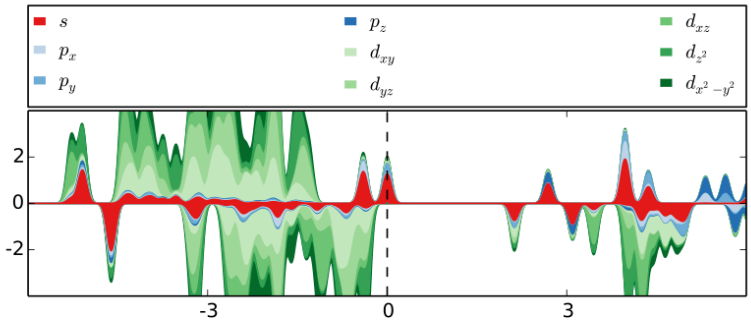

FIG. 87. Projected local density of states for the $Ni_7{}^{2+}$ cluster with a multiplicity of 9 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

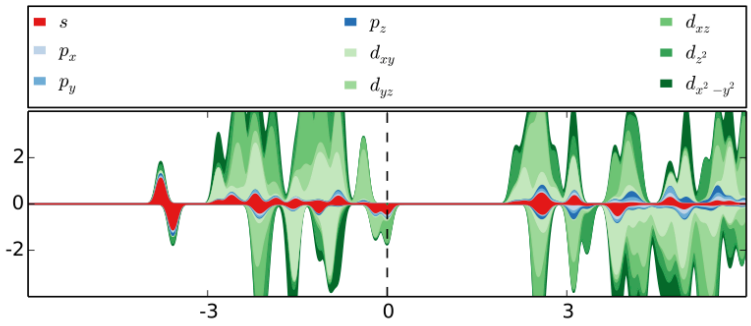

FIG. 88. Projected local density of states for the $V_7{}^{2+}$ cluster with a multiplicity of 12 for the PBE0 exchange-correlation functional. The positive values present the projection values for the spin up Kohn-Sham states and the negative values present the projection values for the spin down Kohn-Sham states. The x axis for this plot is the energy of the states relative to the Fermi energy given in electron Volts.

IV. ADIABATIC IONISATION POTENTIAL

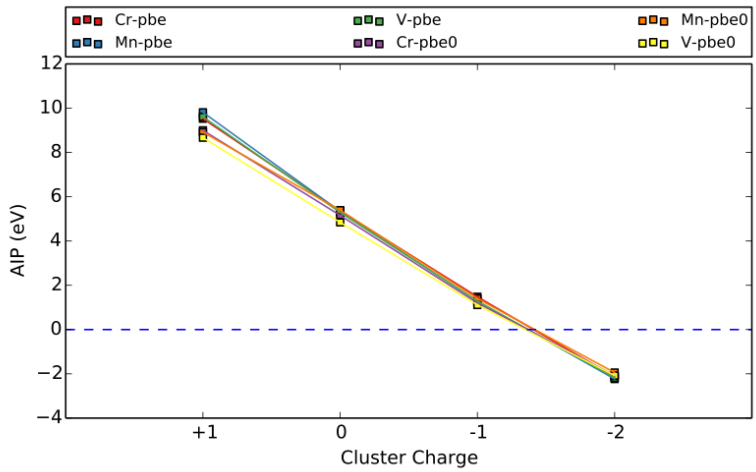

FIG. 89. Adiabatic ionisation potential for the $A_7{}^C$ (A = Cr, Mn, V; C = 0, ±1, ±2) clusters.

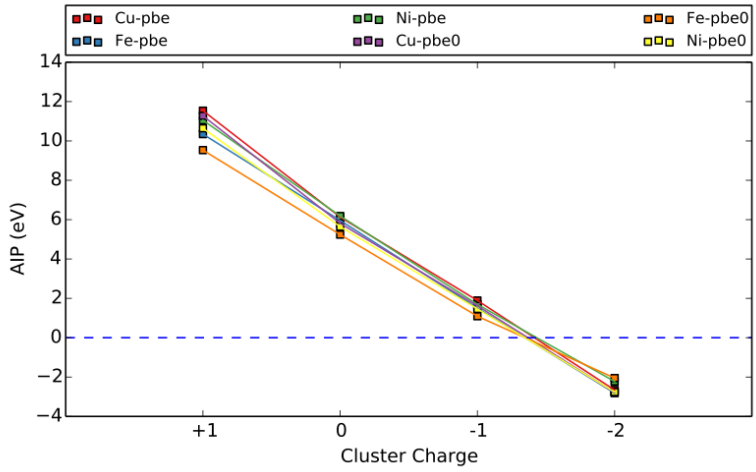

FIG. 90. Adiabatic ionisation potential for the $A_7{}^C$ (A = Fe, Cu, Ni; C = 0, ±1, ±2) clusters.

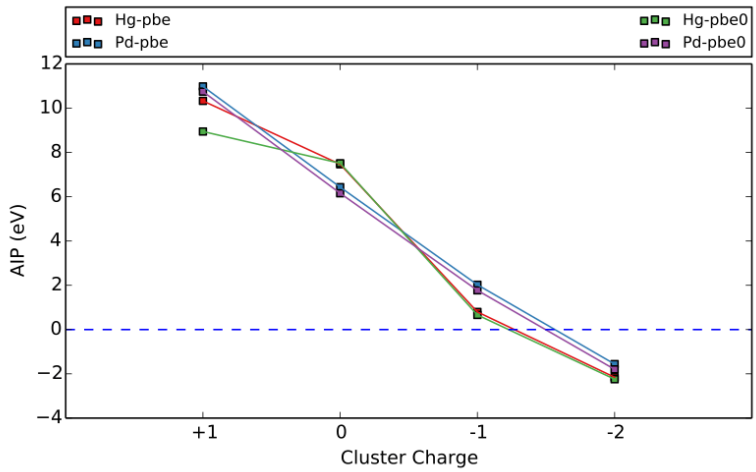

FIG. 91. Adiabatic ionisation potential for the $A_7{}^C$ (A = Hg, Pd; C = 0, ±1, ±2) clusters.

V. ASSIGNED SUPERATOMIC OCCUPANCIES

TABLE I. Assigned superatomic population for the $Cr_7{}^c$ (c = 0, ±1, ±2) clusters for the PBE and PBE0 calculations. These assignments are based off analysis of the PDOS weighting factors, PLDOS and direct visualisation of the Kohn-Sham states.

Cr_7^c		
	PBE	$PBE0$
-2	$1S^2\ 1P^6\ 1D^1$	$1S^2\ 1P^6\ 1D^1$
-1	$1S^2\ 1P^6$	$1S^2\ 1P^6$
0	$1S^2\ 1P^5$	$1S^2\ 1P^5$
$+1$	$1S^2\ 1P^4$	$1S^2\ 1P^4$
$+2$	$1S^2\ 1P^3$	$1S^2\ 1P^3$

TABLE II. Assigned superatomic population for the $Cu_7{}^c$ (c = 0, ±1, ±2) clusters for the PBE and PBE0 calculations. These assignments are based off analysis of the PDOS weighting factors, PLDOS and direct visualisation of the Kohn-Sham states.

Cu_7^c		
	PBE	$PBE0$
-2	$1S^2\ 1P^6\ 1D^1$	$1S^2\ 1P^6\ 1D^1$
-1	$1S^2\ 1P^6$	$1S^2\ 1P^6$
0	$1S^2\ 1P^5$	$1S^2\ 1P^5$
$+1$	$1S^2\ 1P^4$	$1S^2\ 1P^4$
$+2$	$1S^2\ 1P^3$	$1S^2\ 1P^3$

TABLE IV. Assigned superatomic population for the $Hg_7{}^c$ (c = 0, ±1, ±2) clusters for the PBE and PBE0 calculations. These assignments are based off analysis of the PDOS weighting factors, PLDOS and direct visualisation of the Kohn-Sham states.

Hg_7^c		
	PBE	$PBE0$
-2	$1S^2\ 1P^6\ 1D^6\ 2S^2$	$1S^2\ 1P^6\ 1D^6\ 2S^2$
-1	$1S^2\ 1P^6\ 1D^6\ 2S^1$	$1S^2\ 1P^6\ 1D^6\ 2S^1$
0	$1S^2\ 1P^6\ 1D^6$	$1S^2\ 1P^6\ 1D^6$
$+1$	$1S^2\ 1P^6\ 1D^4$	$1S^2\ 1P^6\ 1D^4$
$+2$	$1S^2\ 1P^4\ 1D^4\ 1P^2$	

TABLE III. Assigned superatomic population for the $Pd_7{}^c$ (c = 0, ±1, ±2) clusters for the PBE and PBE0 calculations. These assignments are based off analysis of the PDOS weighting factors, PLDOS and direct visualisation of the Kohn-Sham states.

Pd_7^c		
	PBE	$PBE0$
-2	$1S^2\ 1P^2$	$1S^2\ 1P^2$
-1	$1S^2\ 1P^2$	$1S^2\ 1P^2$
0	$1S^2$	$1S^2$
$+1$	$1S^2$	$1S^2$
$+2$	$1S^2$	$1S^2$

TABLE V. Assigned superatomic population for the $Mn_7{}^c$ (c = 0, ±1, ±2) clusters for the PBE and PBE0 calculations. These assignments are based off analysis of the PDOS weighting factors, PLDOS and direct visualisation of the Kohn-Sham states.

Mn_7^c		
	PBE	$PBE0$
-2	$1S^2\ 1P^6\ 1D^2$	$1S^2\ 1P^6\ 1D^4\ 2S^2\ 2P^2$
-1	$1S^2\ 1P^6\ 1D^3$	$1S^2\ 1P^6\ 1D^4\ 2S^2\ 2P^1$
0	$1S^2\ 1P^6\ 1D^4$	$1S^2\ 1P^6\ 1D^4\ 2S^2$
$+1$	$1S^2\ 1P^6\ 1D^3$	$1S^2\ 1P^6\ 1D^5\ 2S^1$
$+2$	$1S^2\ 1P^5$	$1S^2\ 1P^6\ 1D^3\ 2S^1$

TABLE VI. Assigned superatomic population for the $Fe_7{}^c$ (c = 0, ±1, ±2) clusters for the PBE and PBE0 calculations. These assignments are based off analysis of the PDOS weighting factors, PLDOS and direct visualisation of the Kohn-Sham states.

Fe_7^c		
	PBE	$PBE0$
-2	$1S^2\ 1P^6$	$1S^2\ 1P^6\ 1D^2\ 2S^1$
-1	$1S^2\ 1P^6$	$1S^2\ 1P^6\ 1D^1\ 2S^1$
0	$1S^2\ 1P^6$	$1S^2\ 1P^6$
$+1$	$1S^2\ 1P^6$	$1S^2\ 1P^6$
$+2$	$1S^2\ 1P^5$	$1S^2\ 1P^6$

TABLE VII. Assigned superatomic population for the $Ni_7{}^c$ (c = 0, ±1, ±2) clusters for the PBE and PBE0 calculations. These assignments are based off analysis of the PDOS weighting factors, PLDOS and direct visualisation of the Kohn-Sham states.

Ni_7^c		
	PBE	$PBE0$
-2	$1S^2\ 1P^6$	$1S^2\ 1P^6$
-1	$1S^2\ 1P^5$	$1S^2\ 1P^6$
0	$1S^2\ 1P^4$	$1S^2\ 1P^5$
$+1$	$1S^2\ 1P^2$	$1S^2\ 1P^4$
$+2$	$1S^2\ 1P^2$	$1S^2\ 1P^3$

TABLE VIII. Assigned superatomic population for the $V_7{}^c$ (c = 0, ±1, ±2) clusters for the PBE and PBE0 calculations. These assignments are based off analysis of the PDOS weighting factors, PLDOS and direct visualisation of the Kohn-Sham states.

V_7^c		
	PBE	$PBE0$
-2	$1S^2\ 2S^2\ 1P^5$	$1S^2\ 1P^6\ 1D^1$
-1	$1S^2\ 2S^2\ 1P^4$	$1S^2\ 1P^6$
0	$1S^2\ 2S^2 1P^4$	$1S^2\ 1P^5$
$+1$	$1S^2\ 2S^2 1P^4$	$1S^2\ 1P^4$
$+2$	$1S^2\ 2S^2 1P^4$	$1S^2\ 1P^3$