Robust Magnetic Moments on Impurities in Metallic Clusters: Localized Magnetic States in Superatoms

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Supplementary information

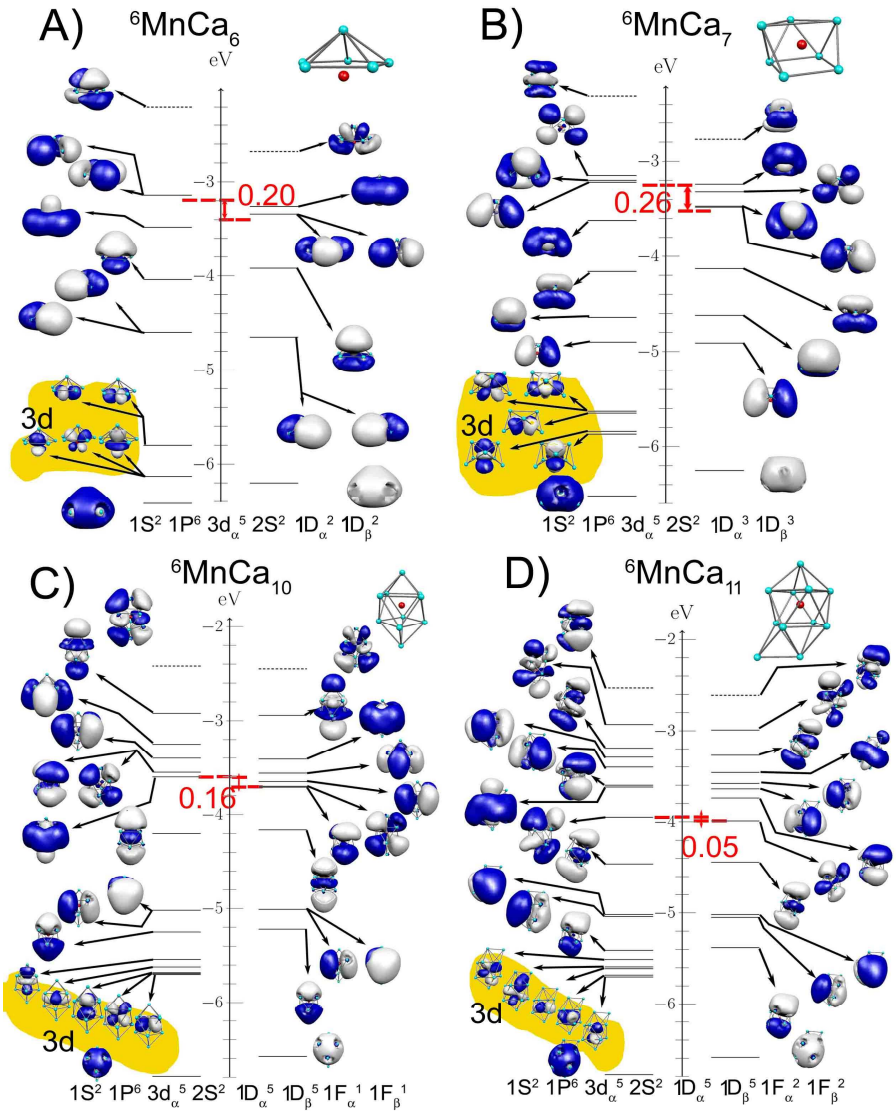

Figure S1. The one-electron energy levels and molecular orbital wavefunction isosurfaces for A) $^6MnCa_6$, B) $^6MnCa_7$, C) $^6MnCa_{10}$, and D) $^6MnCa_{11}$

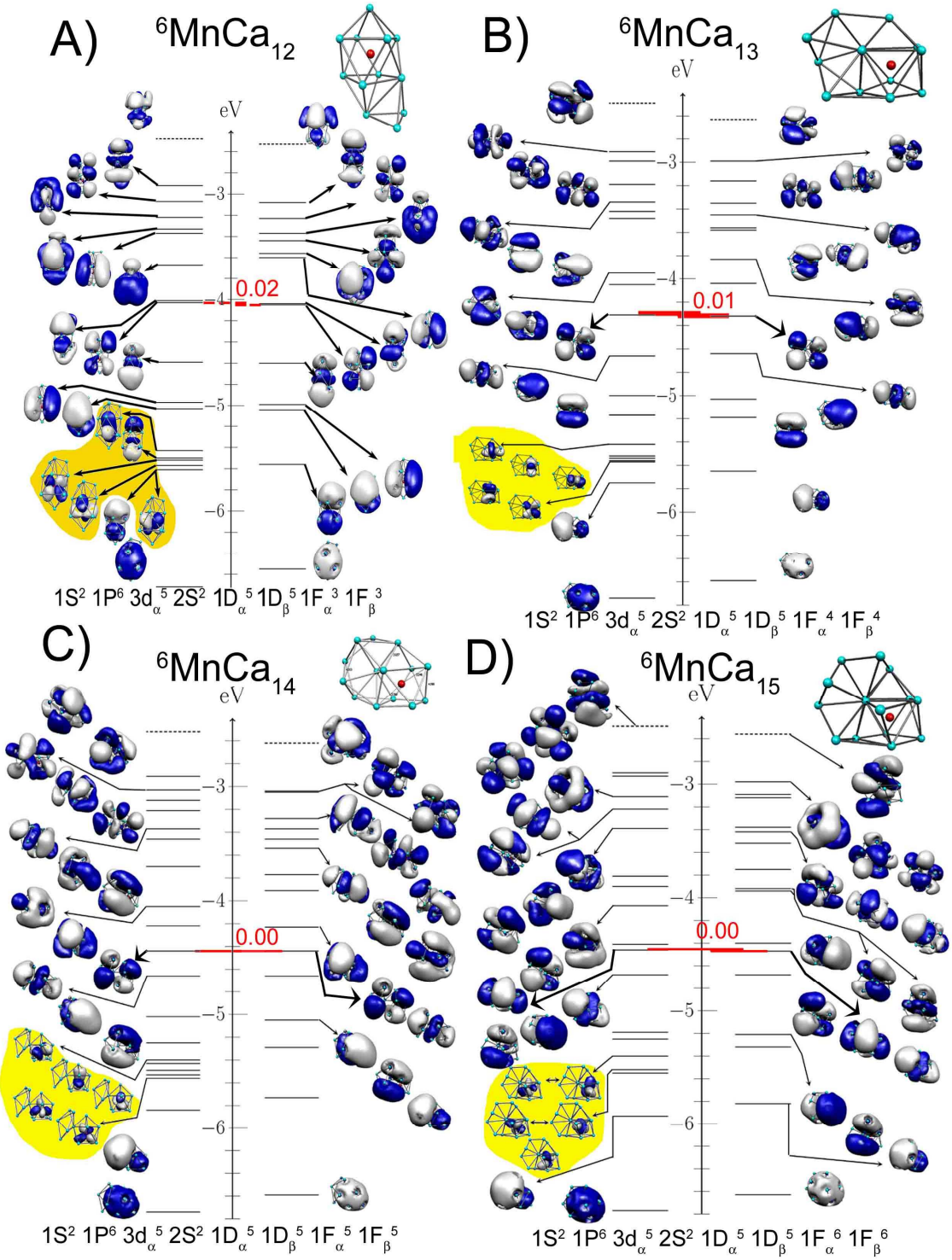

Figure S2. The one-electron energy levels and molecular orbital wavefunction isosurfaces for A) $^6MnCa_{12}$, B) $^6MnCa_{13}$, C) $^6MnCa_{14}$, and D) $^6MnCa_{15}$

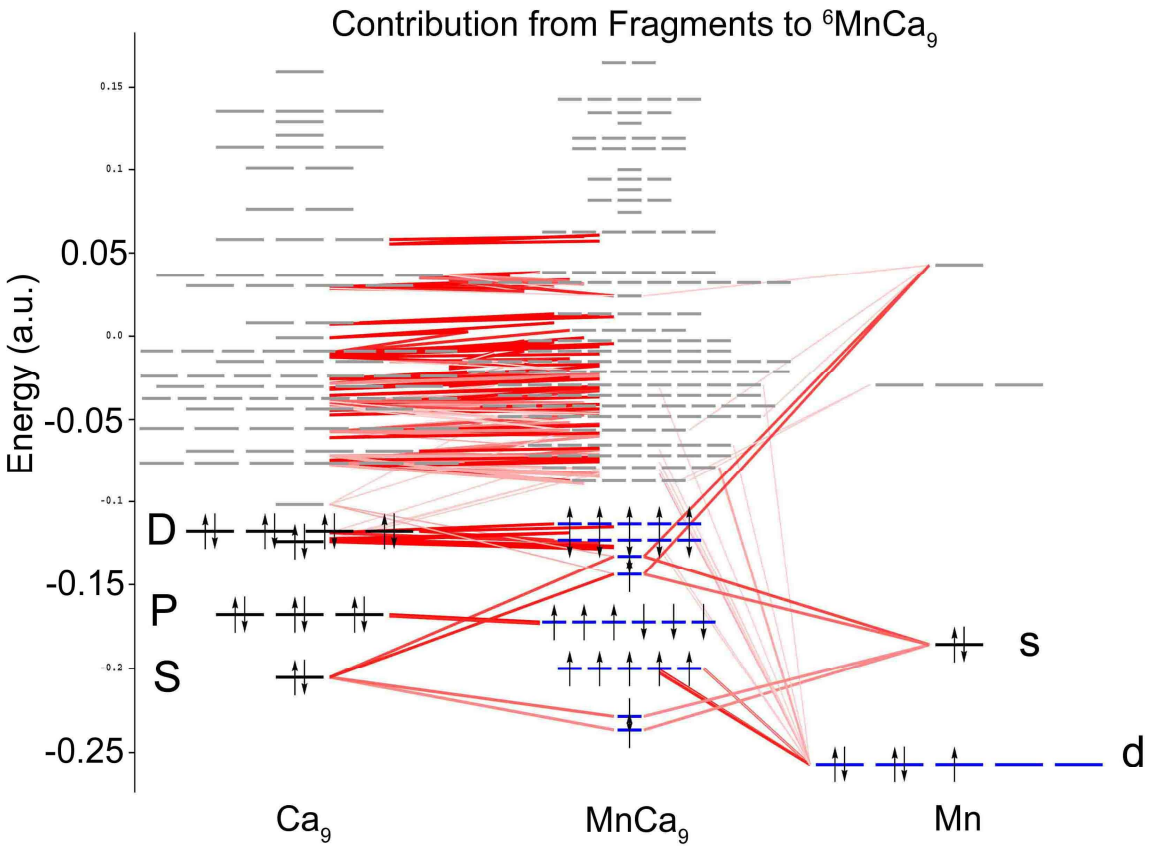

Figure S3. Decomposition of molecular orbitals of $^6MnCa_9$ in the center, into two fragments. In the left is the Ca_9 fragment and in the right is the Mn atom.

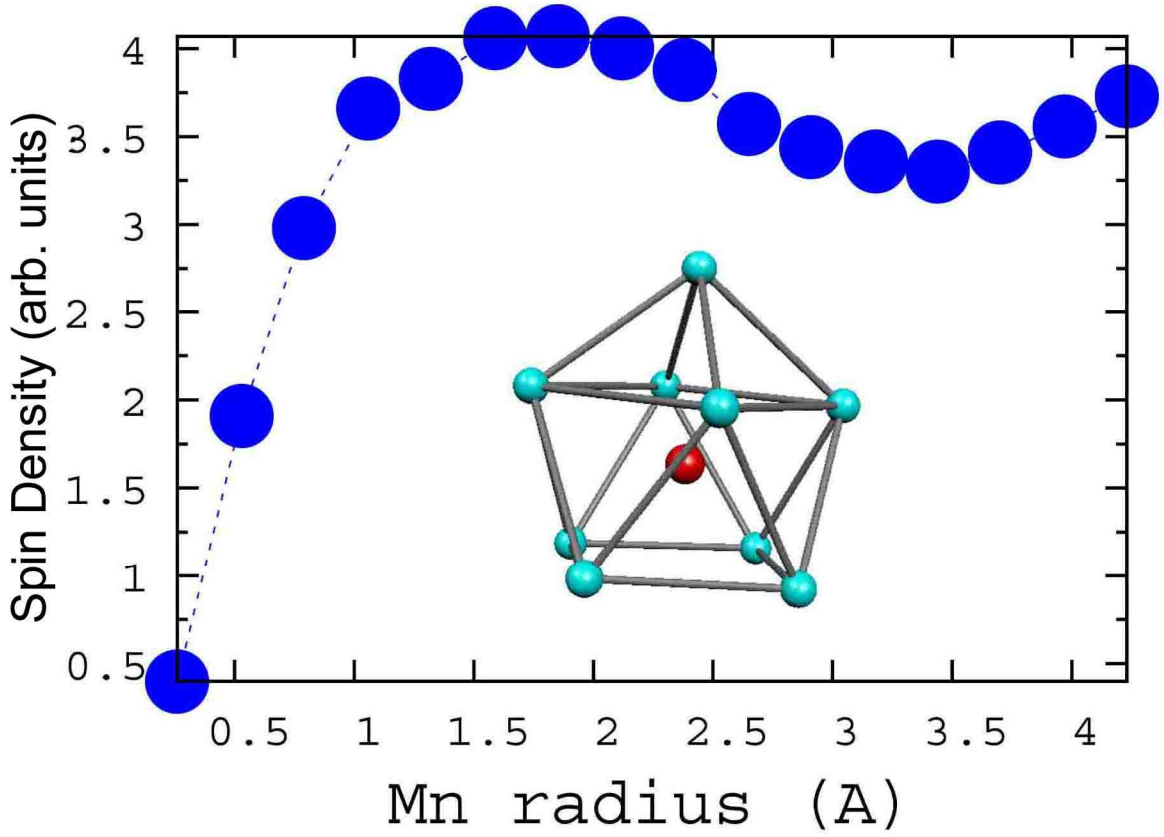

Figure S4. Spin polarization for $MnCa_9$ as a function of the distance of Mn atom.

Table S1. Magnetic anisotropy for various clusters.

Cluster	Anisotropy (K)
$MnCa_8$	1.93
$MnCa_9$	0.03
$MnCa_9$ dimer (AF)	1.65
$MnCa_9$ dimer (FE)	2.42