Supporting information for: First-principles calculations of the electronic structure and bonding in metal cluster-fullerene materials considered within the superatomic framework

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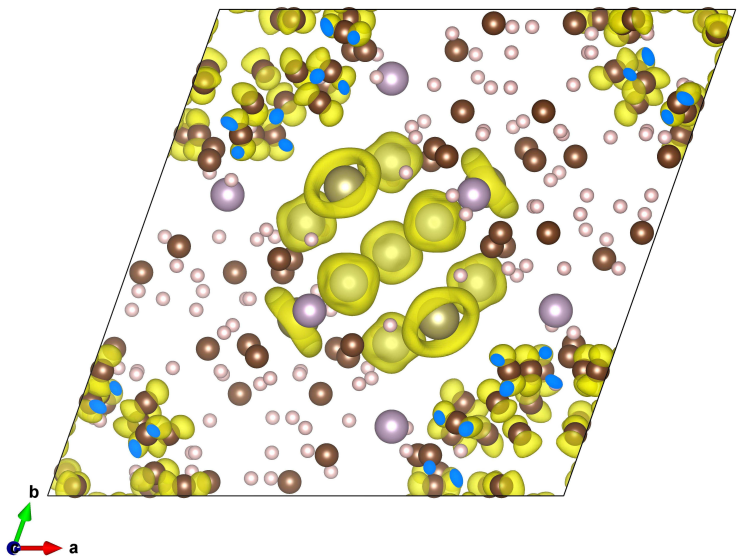

Figure S1: Band decomposed charge density for one of the three highest occupied bands in $[Ni_9Te_6(PEt_3)_8]C_{60}$.

As described in the main article, Figs. S2-S4 show the angular momentum-projected DOS for spherical harmonic functions centered at the cluster center for the transition metal clusters, in both the bulk compound and for the free clusters. The electronic structure of free clusters were calculated for charges that range from 0 to 2. Figs. S2-S4 reveal that angular momentum-projected DOS for the free clusters show strong similarities, whenever the applied charge in the cluster is closest to the charge observed in the compound by a Bader analysis.

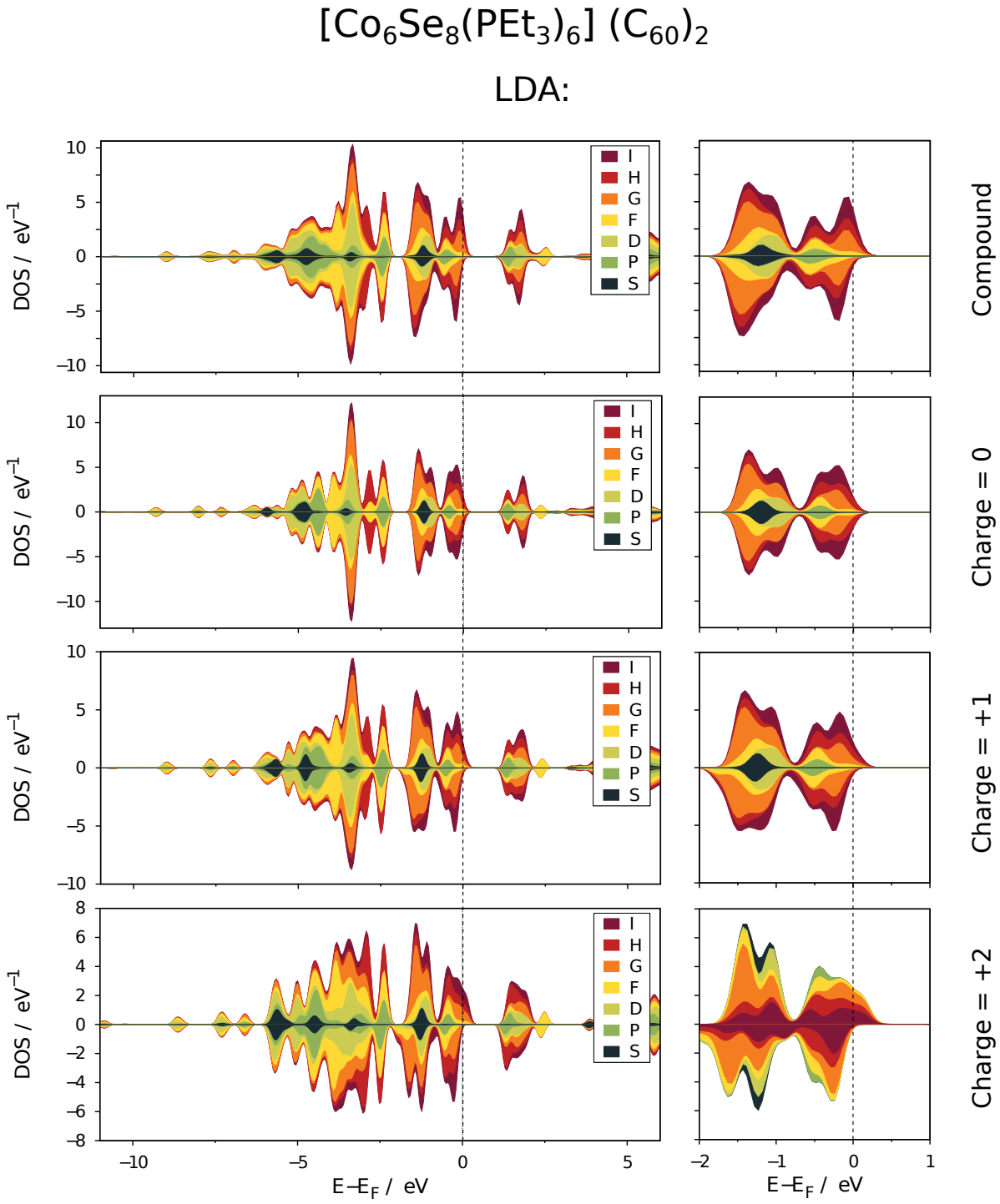

Figure S2: Superatomic character for the compound $[Co_6Se_8(PEt_3)_6][C_{60}]_2$ and its corresponding ligand-protected metal clusters for charges $q = 0, 1, 2$. Contributions to the projected DOS are shown in a stacked view, such that the height of the DOS represents the total DOS.

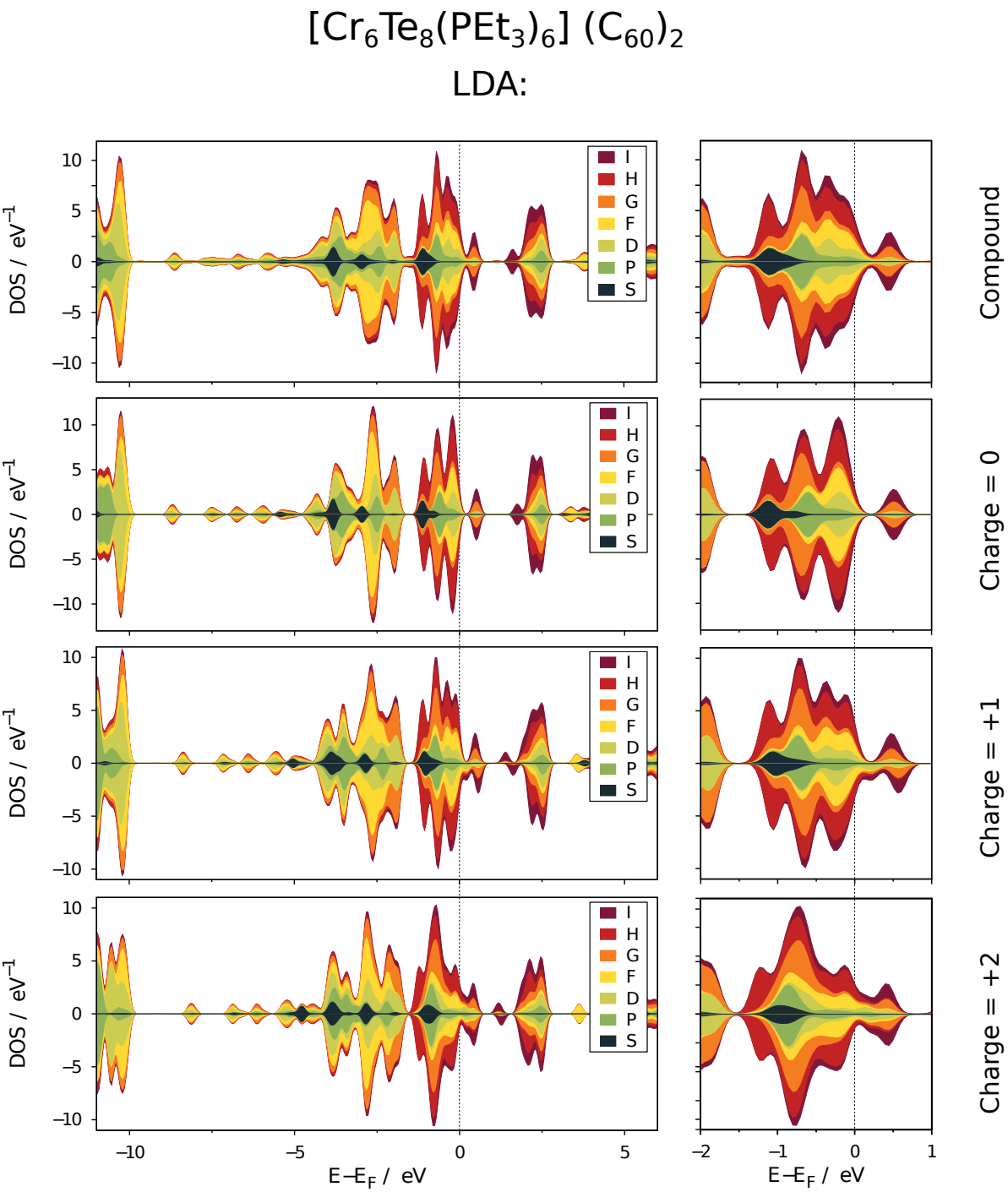

Figure S3: Superatomic character for the compound $[Cr_6Te_8(PEt_3)_6][C_{60}]_2$ and its corresponding ligand-protected metal clusters for charges $q = 0, 1, 2$. Contributions to the projected DOS are shown in a stacked view, such that the height of the DOS represents the total DOS.

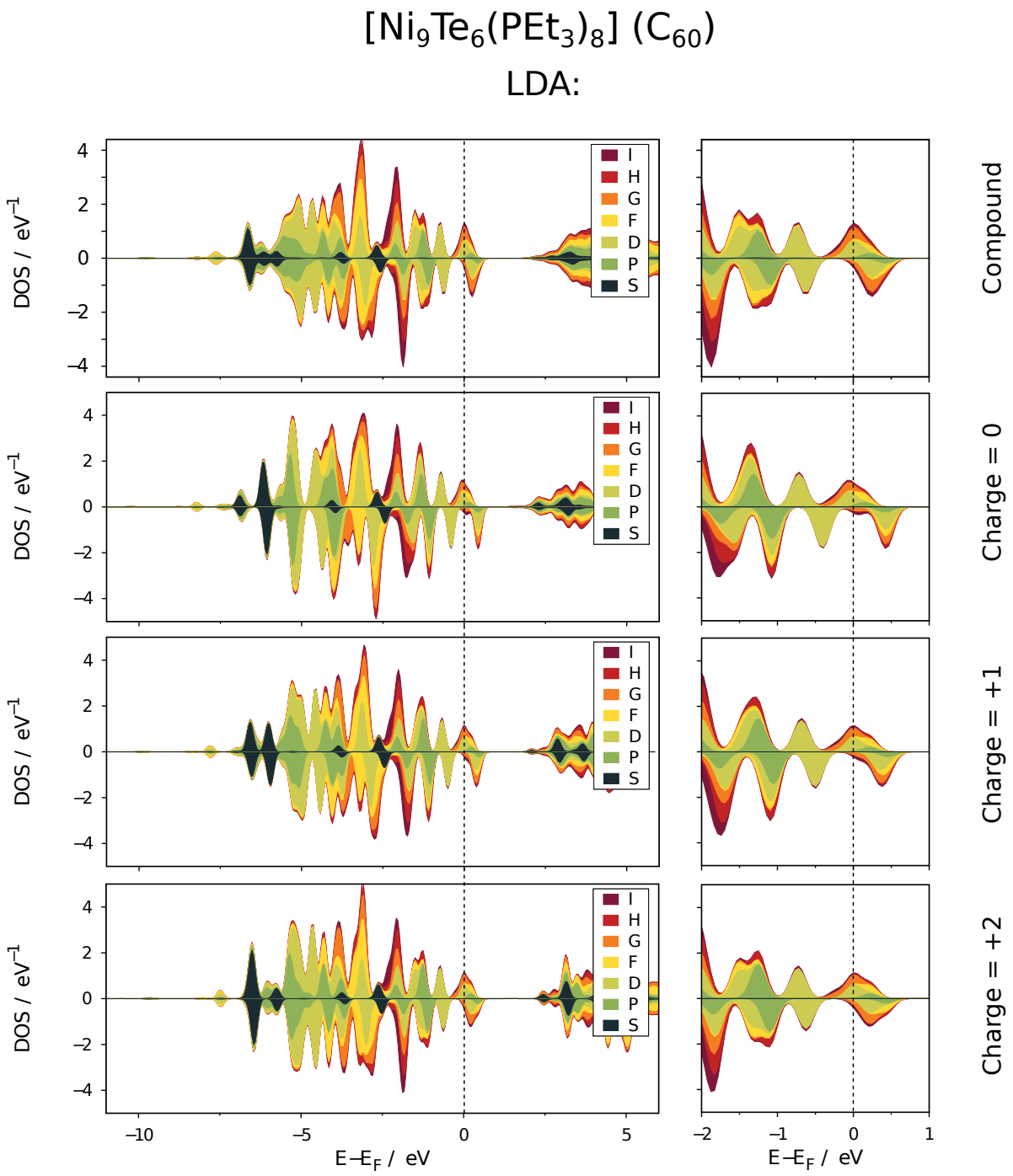

Figure S4: Superatomic character for the compound $[Ni_9Te_6(PEt_3)_8]C_{60}$ and its corresponding ligand-protected metal clusters for charges $q = 0, 1, 2$. Contributions to the projected DOS are shown in a stacked view, such that the height of the DOS represents the total DOS.