The list of calculation results of the Mulliken Population Analysis in each superatomic-like X@Ga_{12} cluster model used for the one-electron calculation (DV-Xα molecular orbital method).

※ The length of the horizontal axis shows the relative proportions of the atomic orbitals, and the vertical axis shows the serial numbers of the molecular orbitals corresponding to each superatomic-like orbital of the X@Ga_{12} cluster.

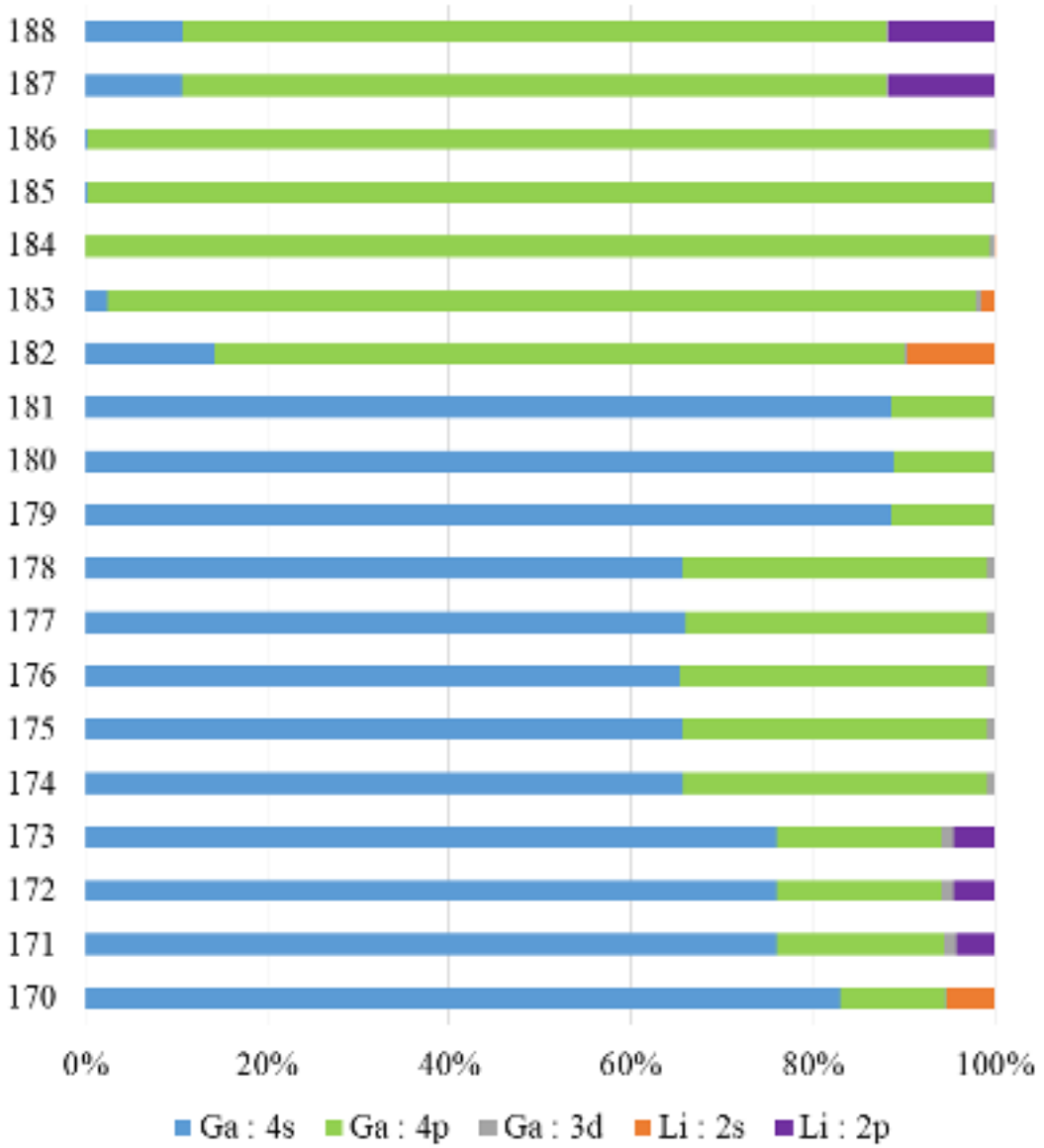

Figure S1. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Li@Ga_{12}$ cluster (interatomic Li-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

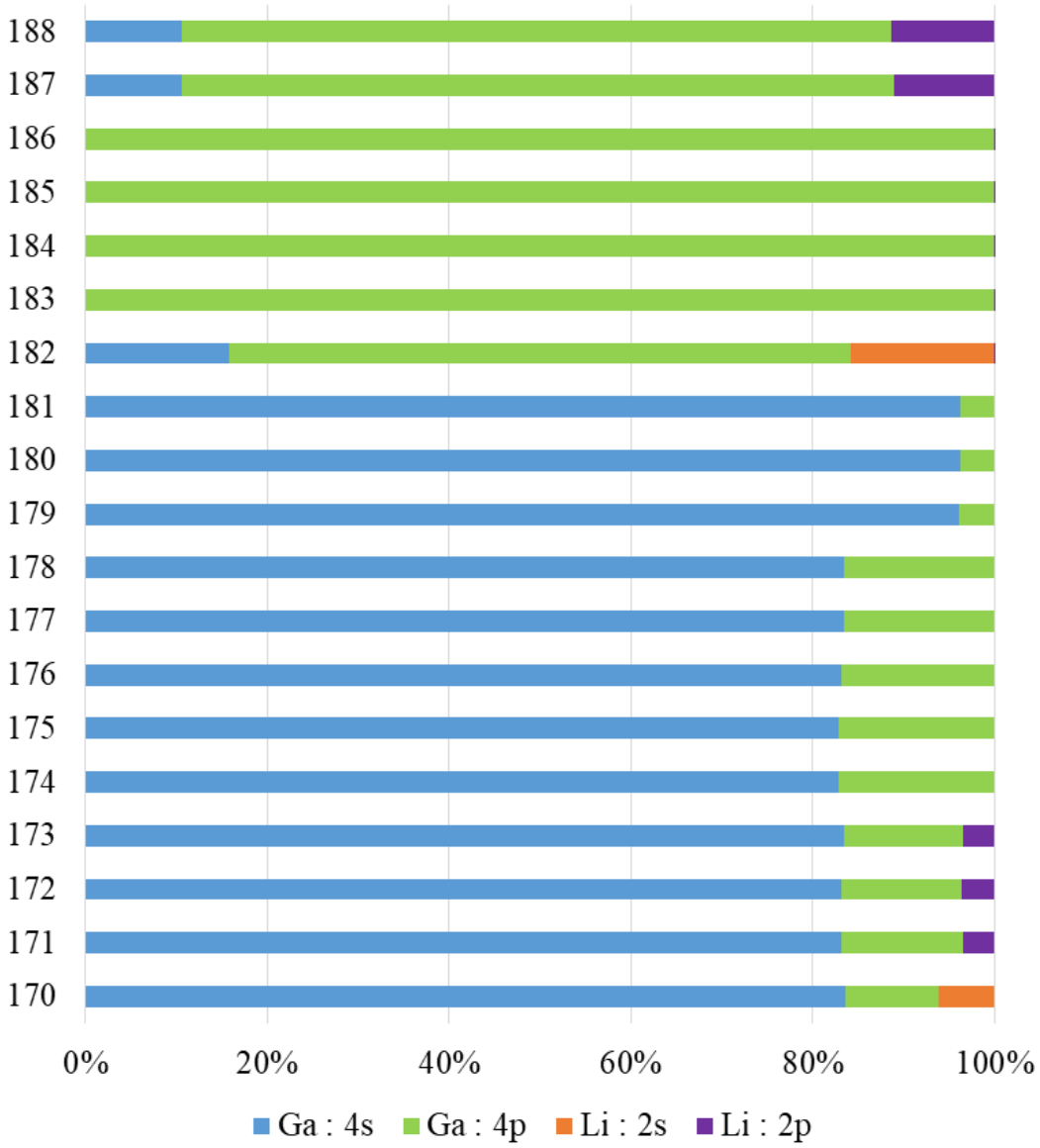

Figure S2. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Li@Ga_{12}$ cluster (interatomic Li-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

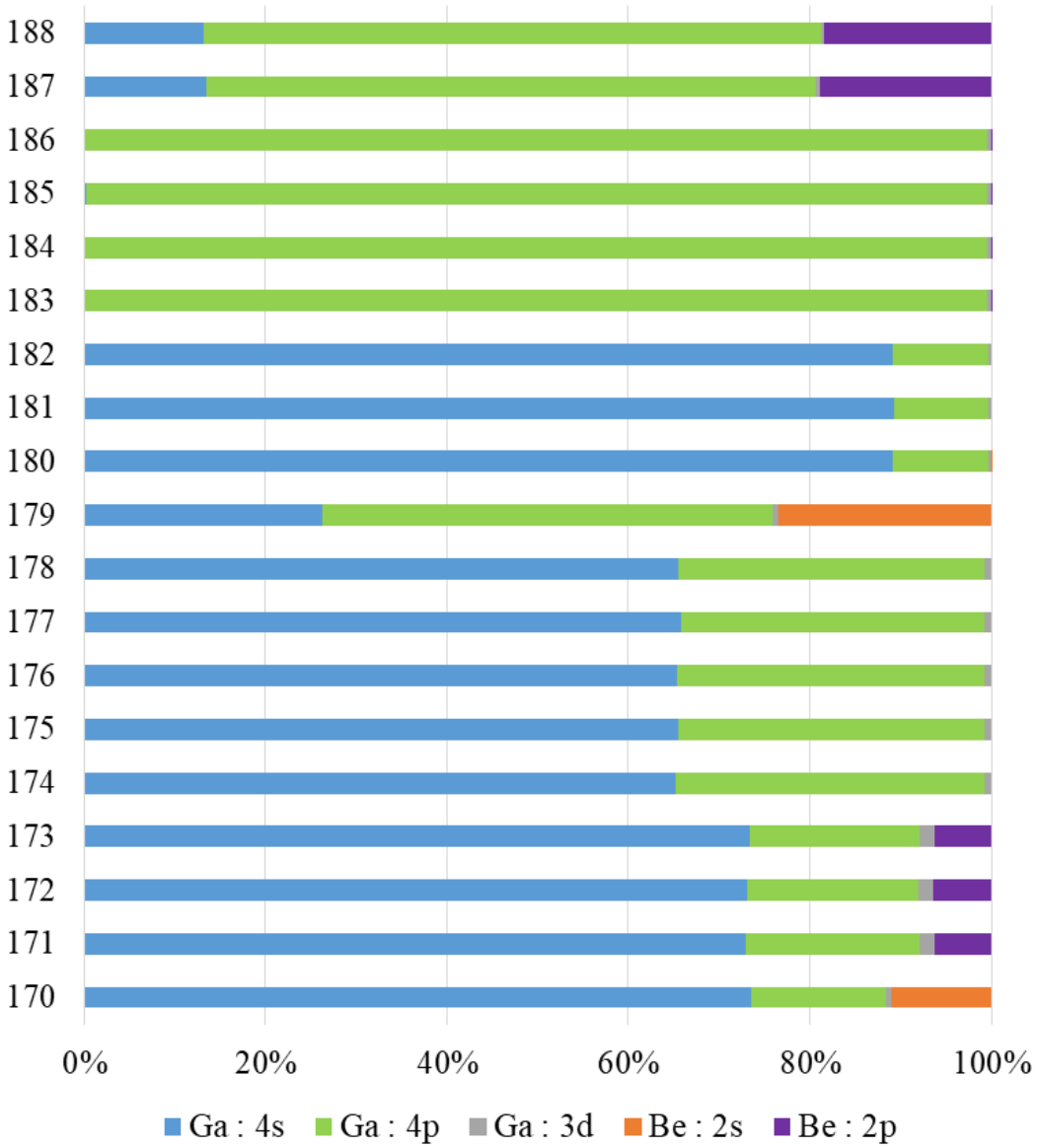

Figure S3. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Be@Ga_{12}$ cluster (interatomic Be-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

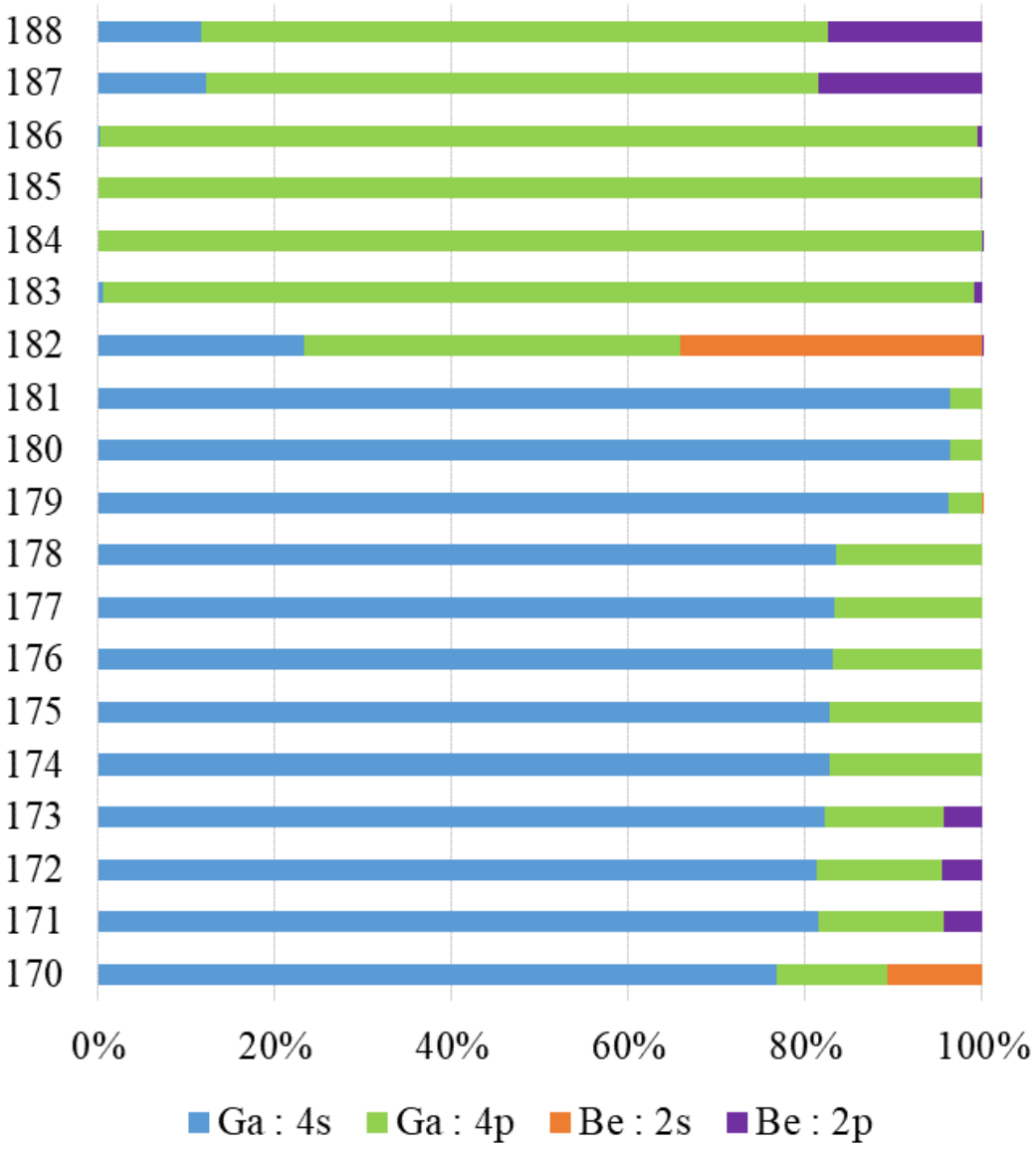

Figure S4. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Be@Ga_{12}$ cluster (interatomic Be-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

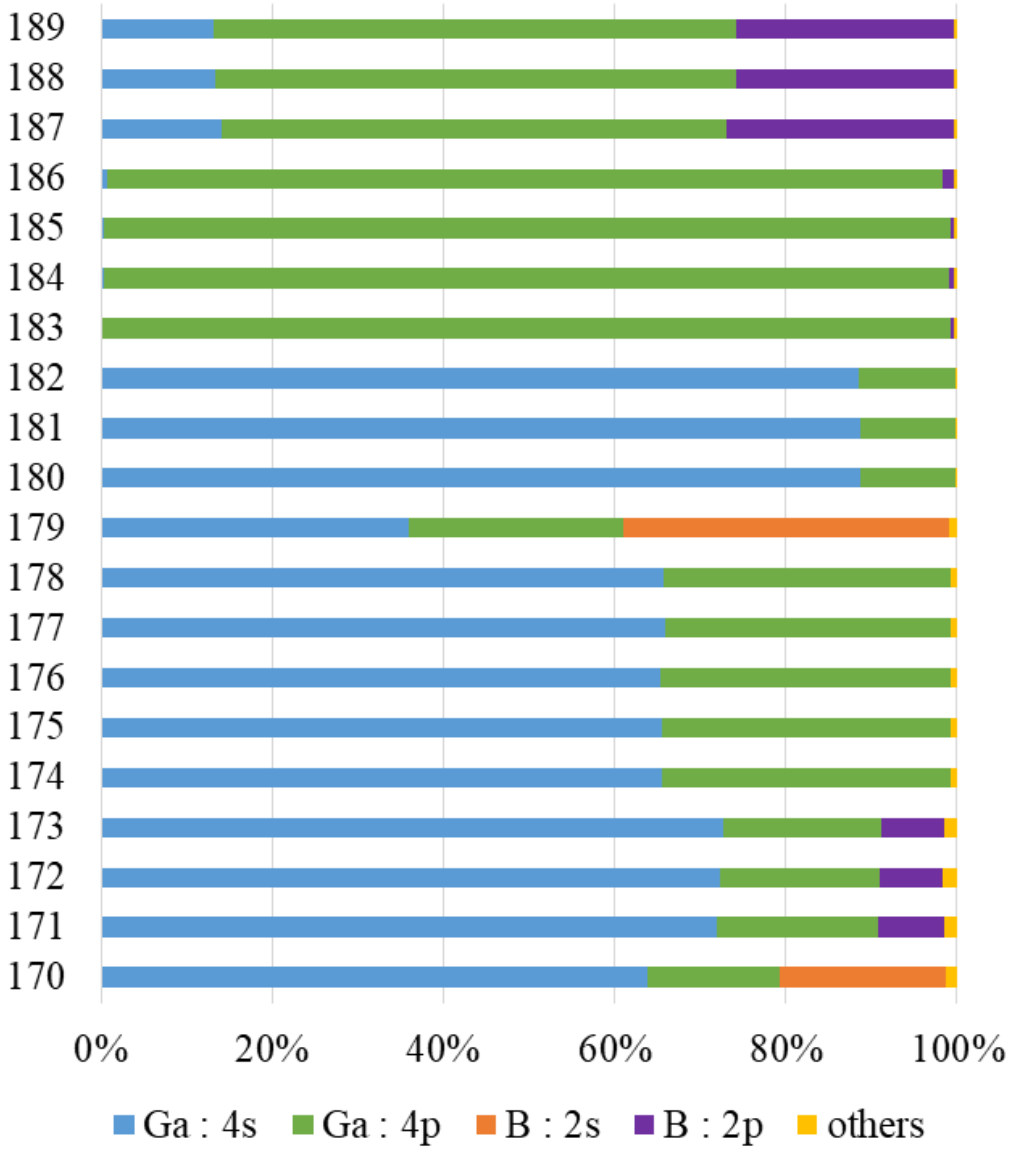

Figure S5. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the B@Ga_{12} cluster (interatomic B-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

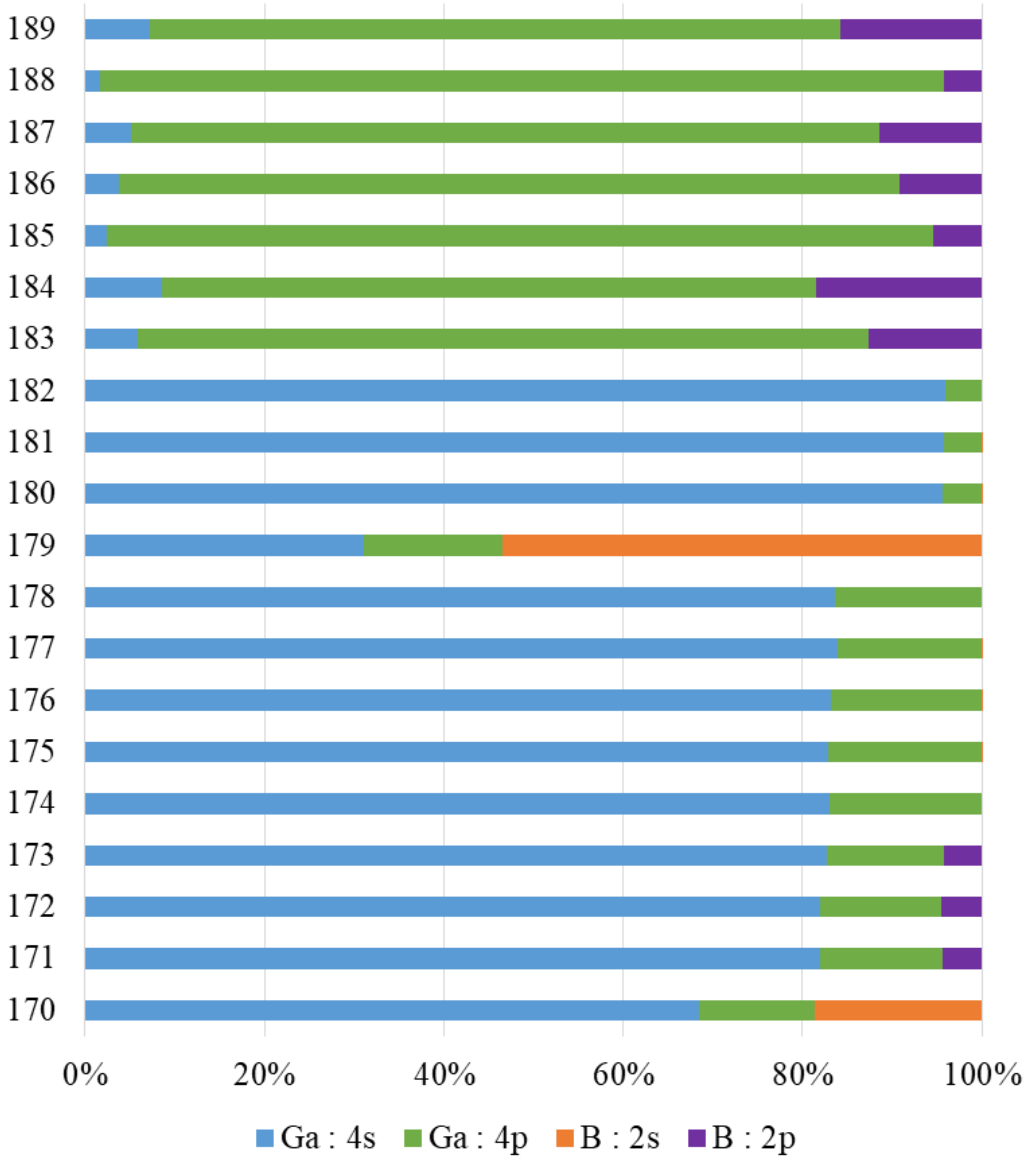

Figure S6. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the B@Ga_{12} cluster (interatomic B-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

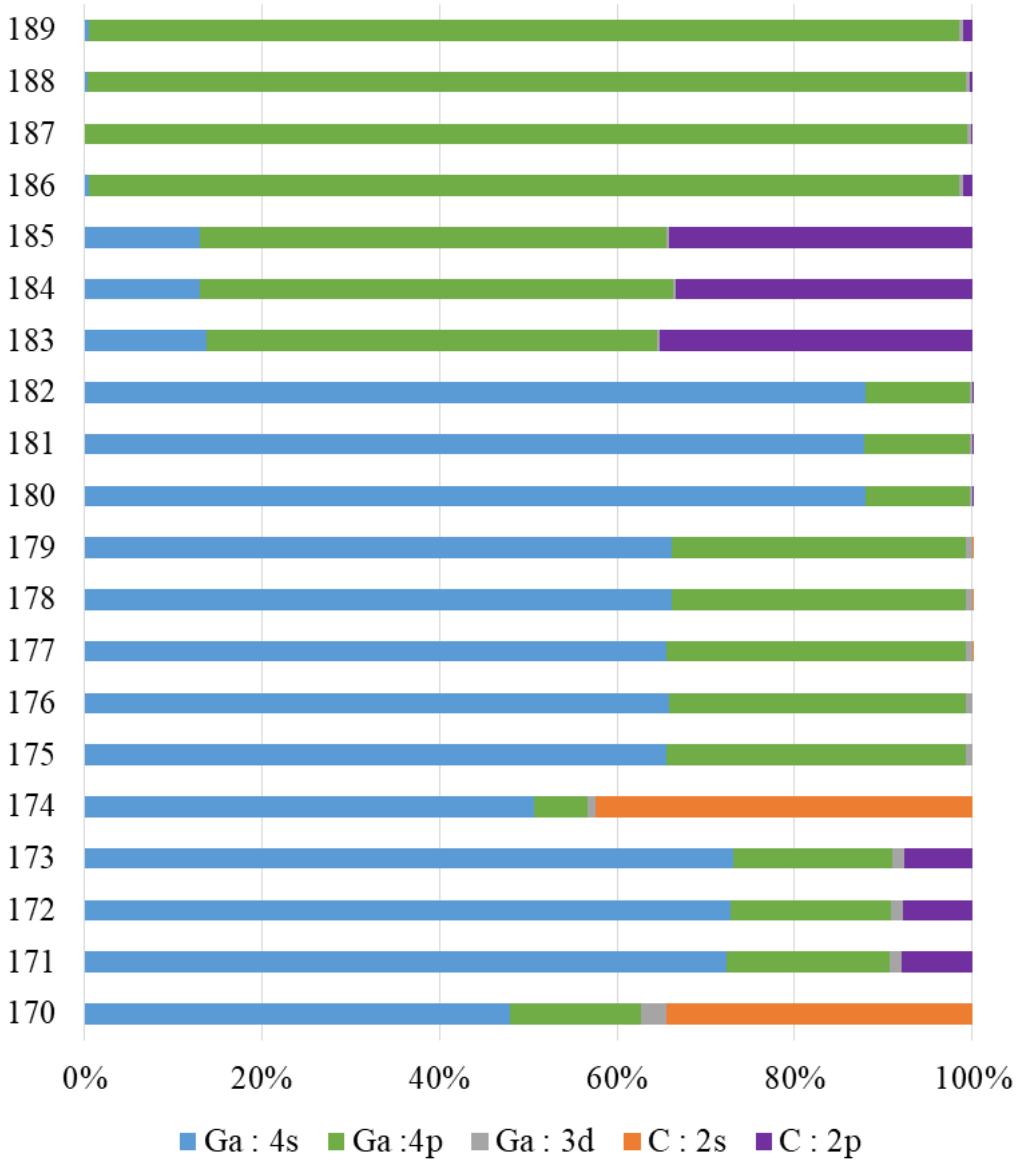

Figure S7. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the C@Ga_{12} cluster (interatomic C-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

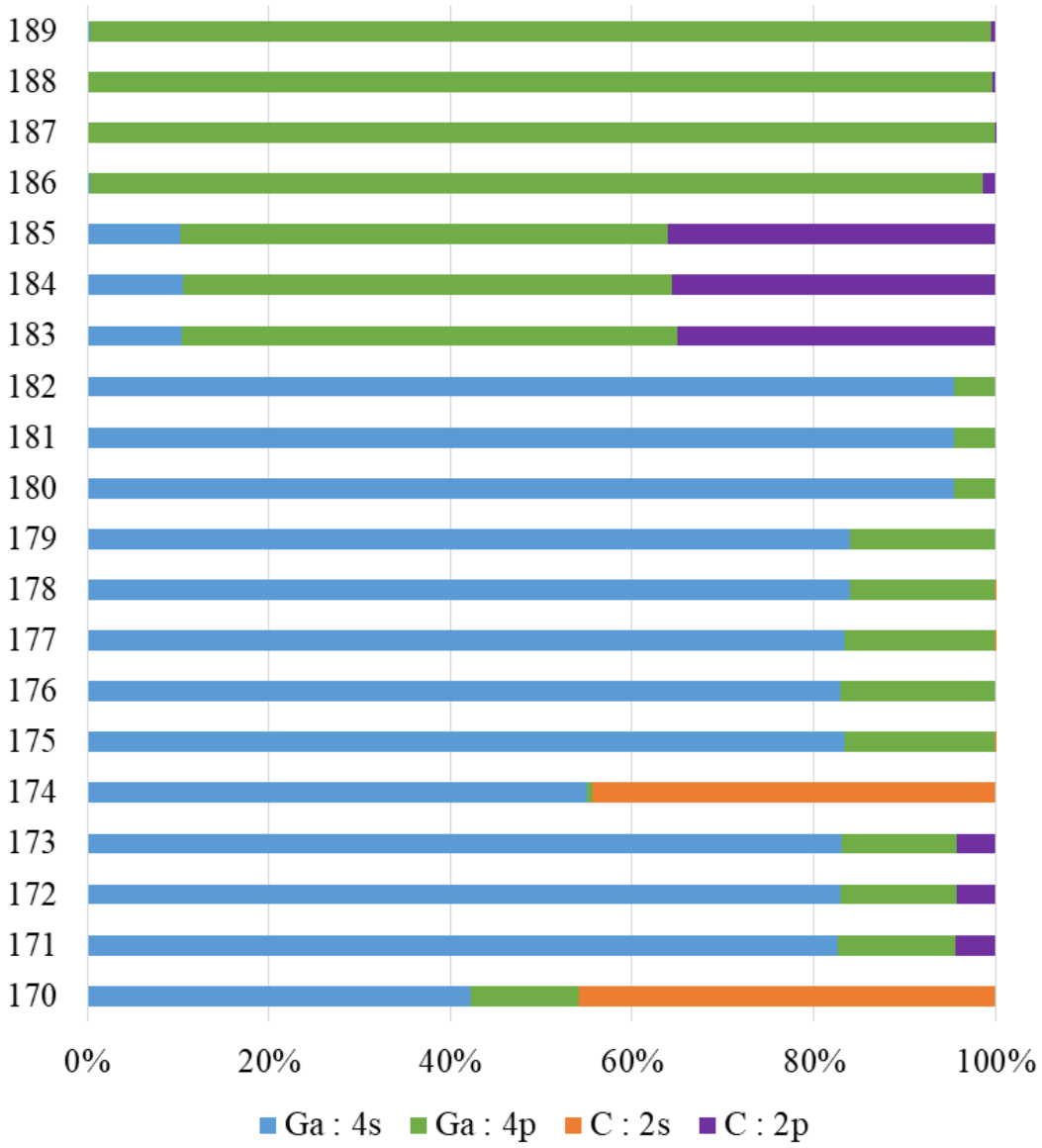

Figure S8. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the C@Ga_{12} cluster (interatomic C-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

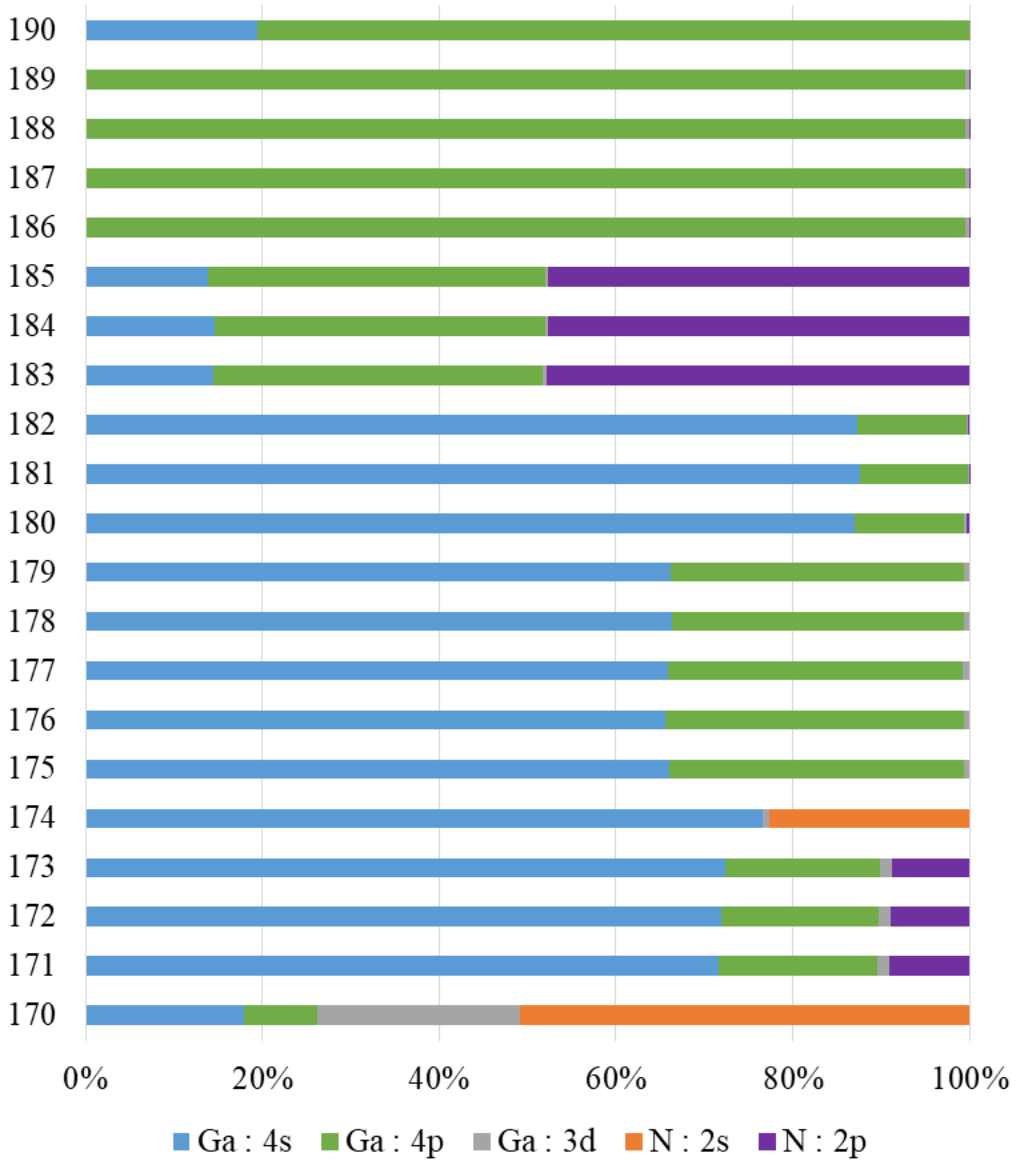

Figure S9. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $N@Ga_{12}$ cluster (interatomic N-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

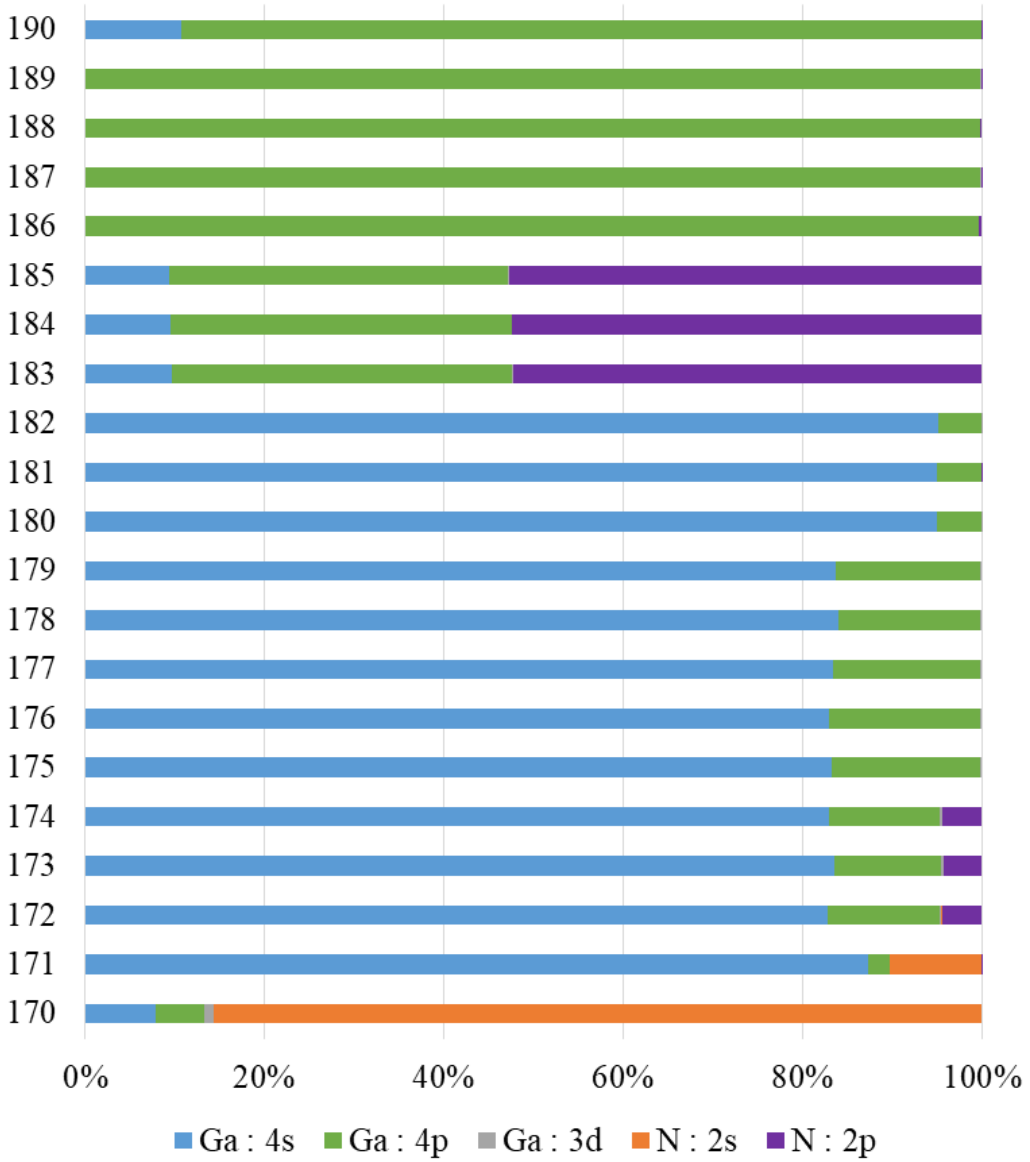

Figure S10. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $N@Ga_{12}$ cluster (interatomic N-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

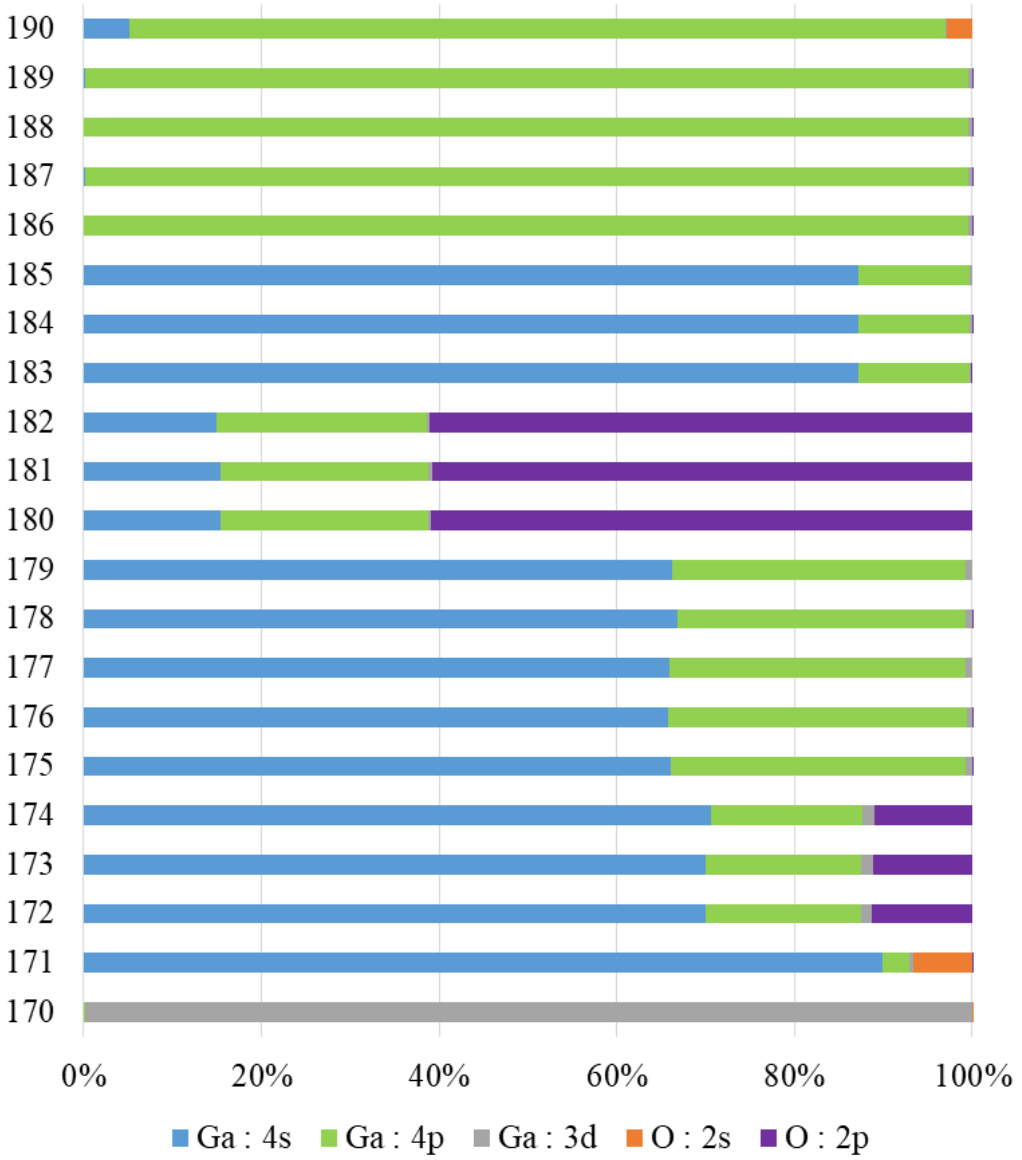

Figure S11. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the O@Ga_{12} cluster (interatomic O-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

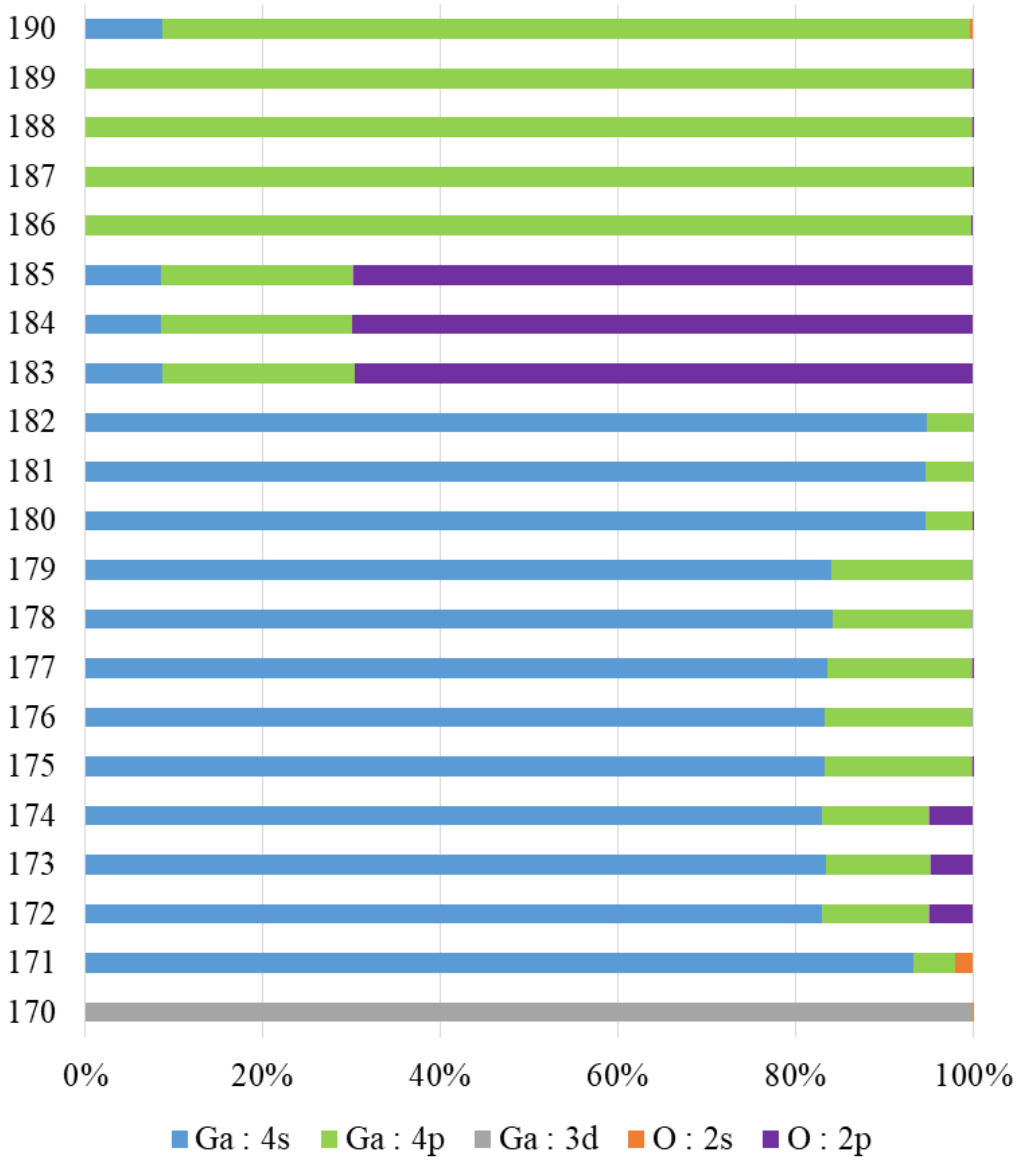

Figure S12. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $O@Ga_{12}$ cluster (interatomic O-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

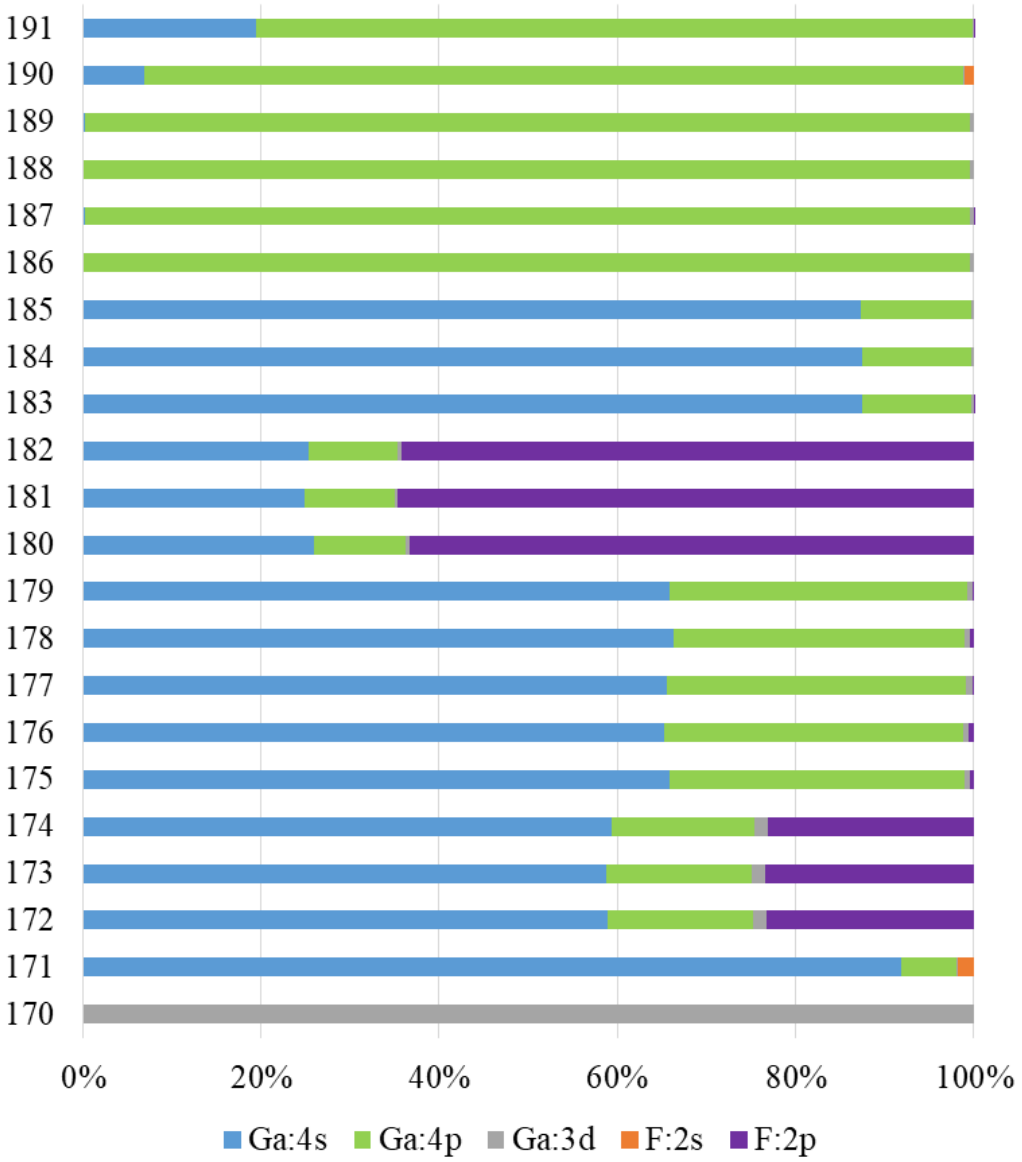

Figure S13. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the F@Ga_{12} cluster (interatomic F-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

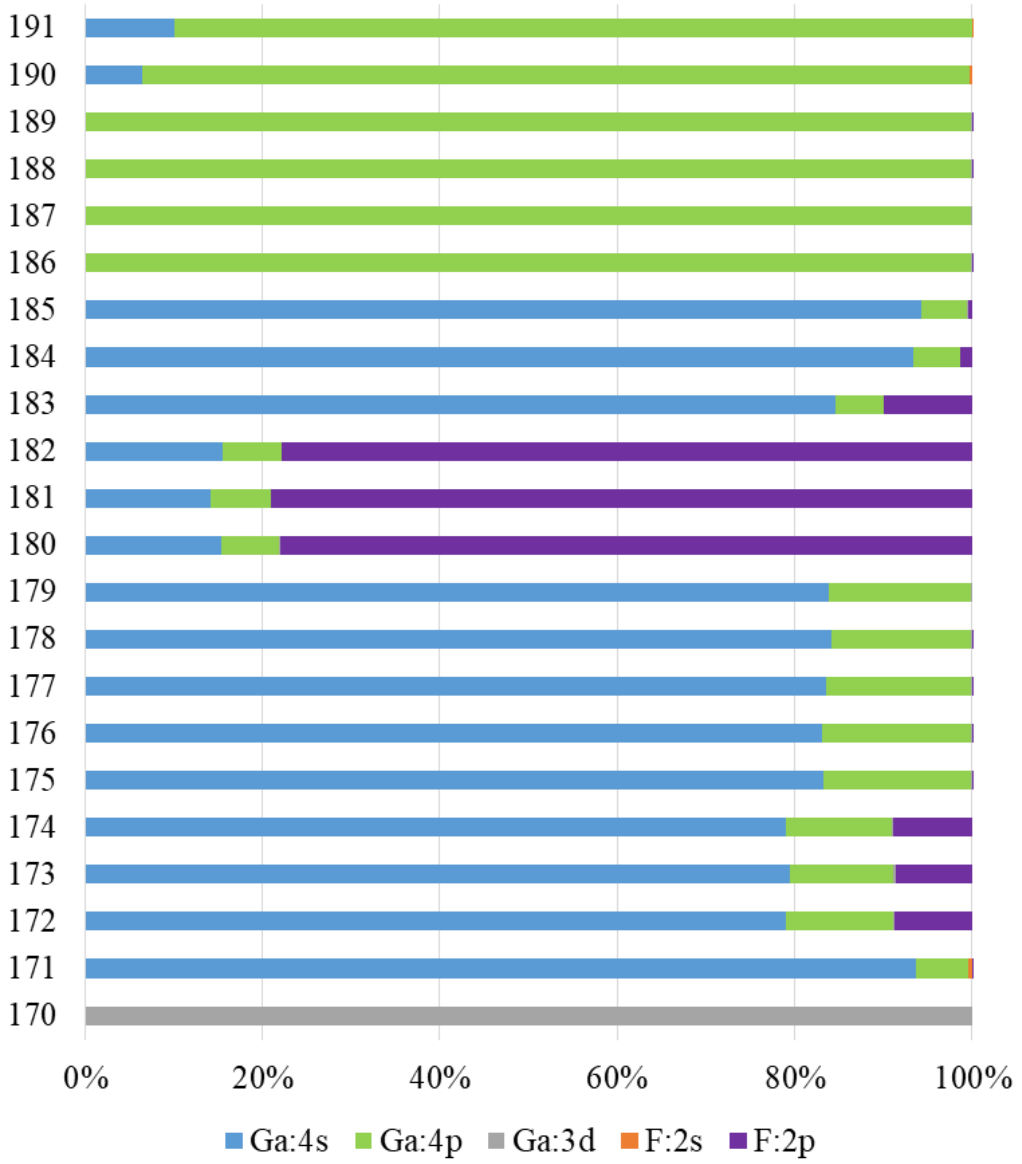

Figure S14. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the F@Ga_{12} cluster (interatomic F-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

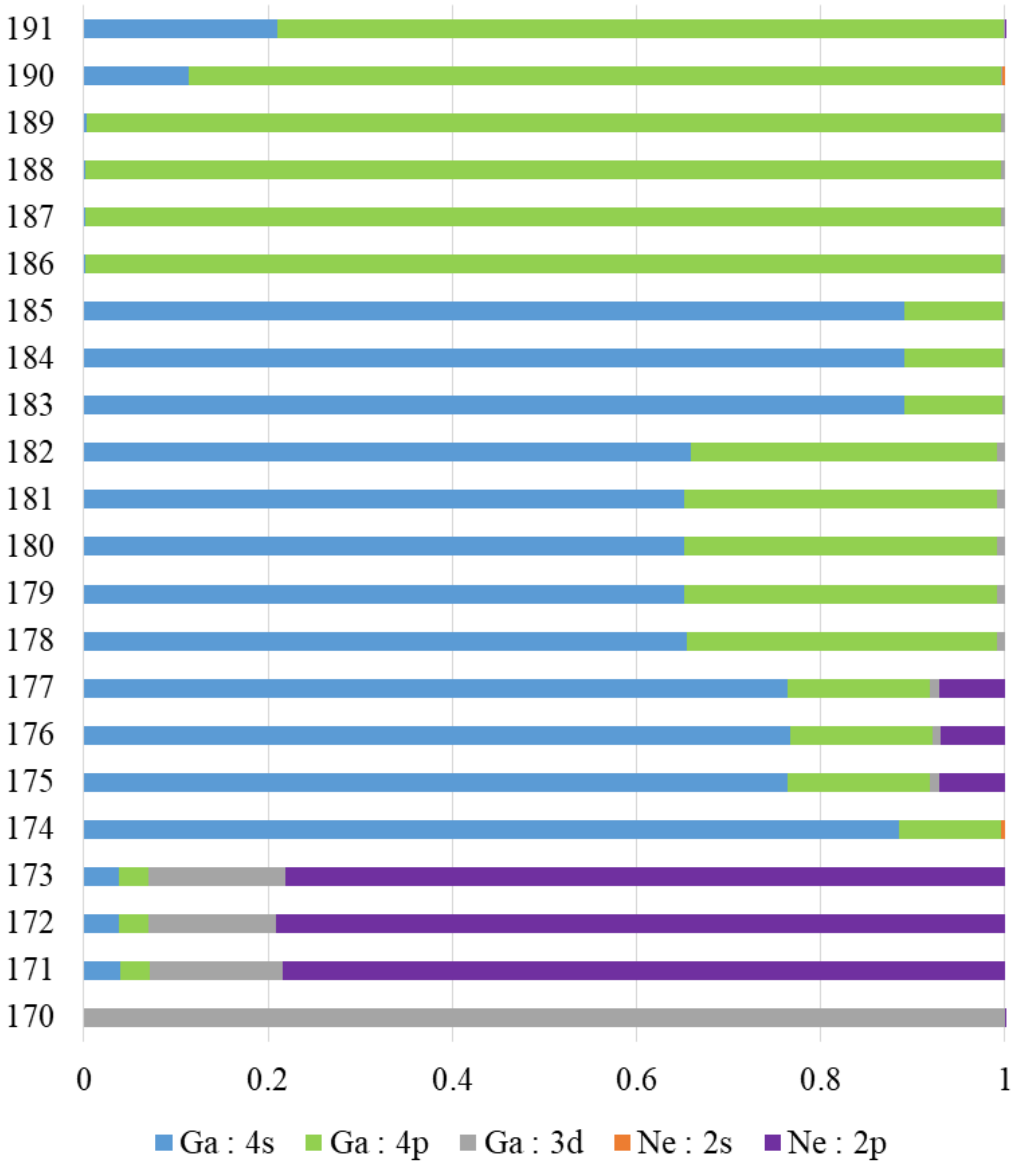

Figure S15. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the Ne@Ga_{12} cluster (interatomic Ne-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

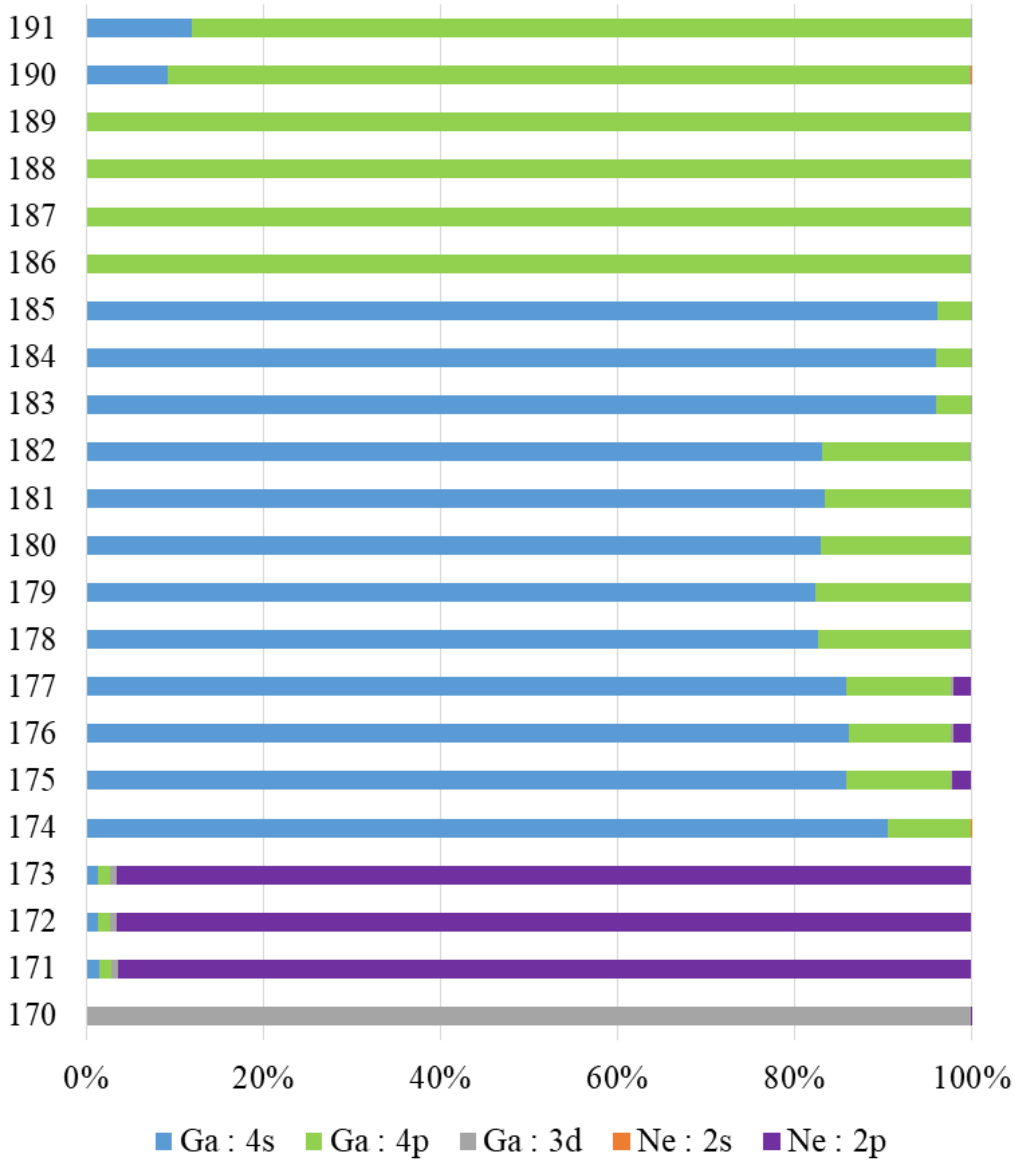

Figure S16. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the Ne@Ga_{12} cluster (interatomic Ne-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

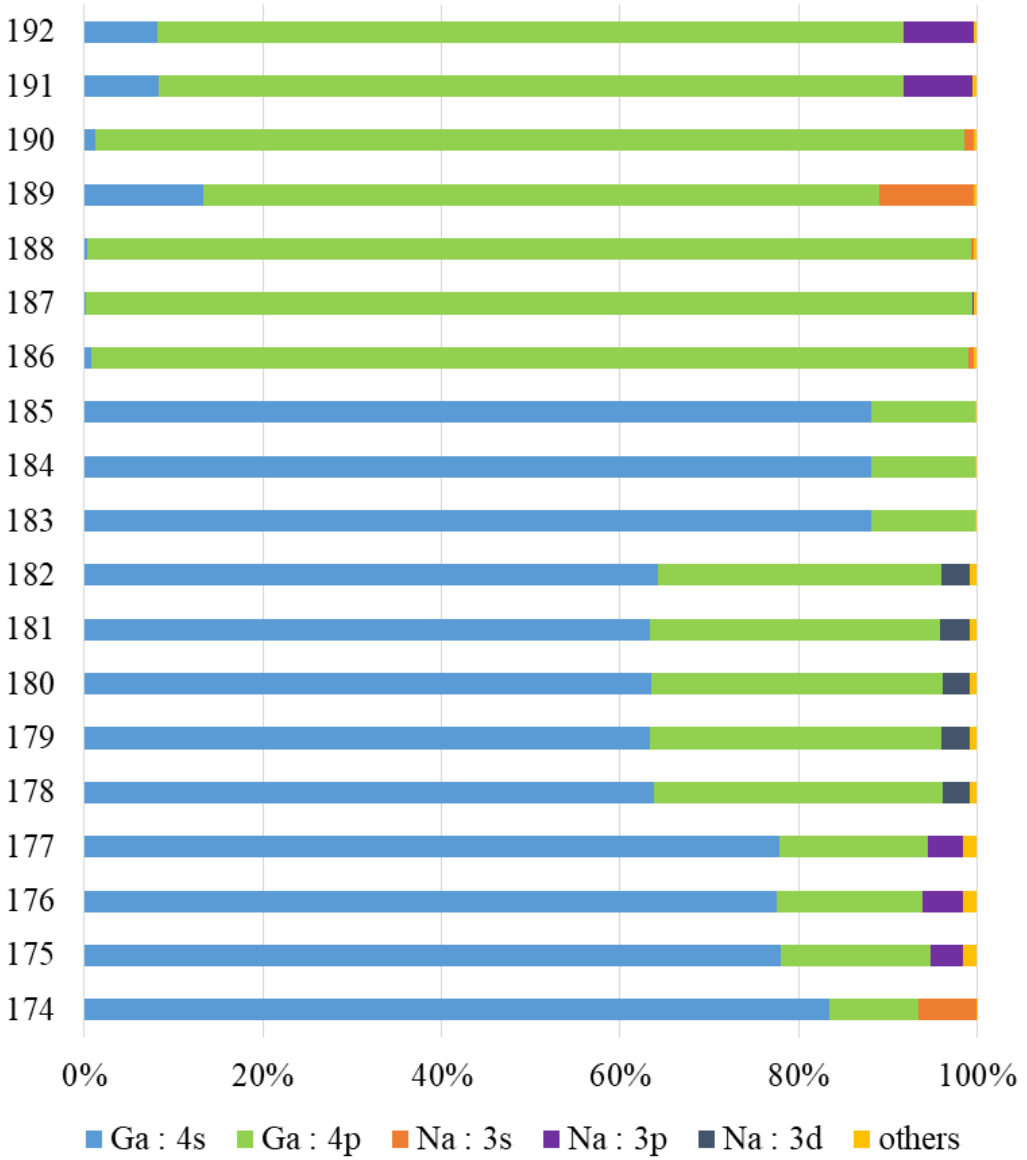

Figure S17. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Na@Ga_{12}$ cluster (interatomic Na-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

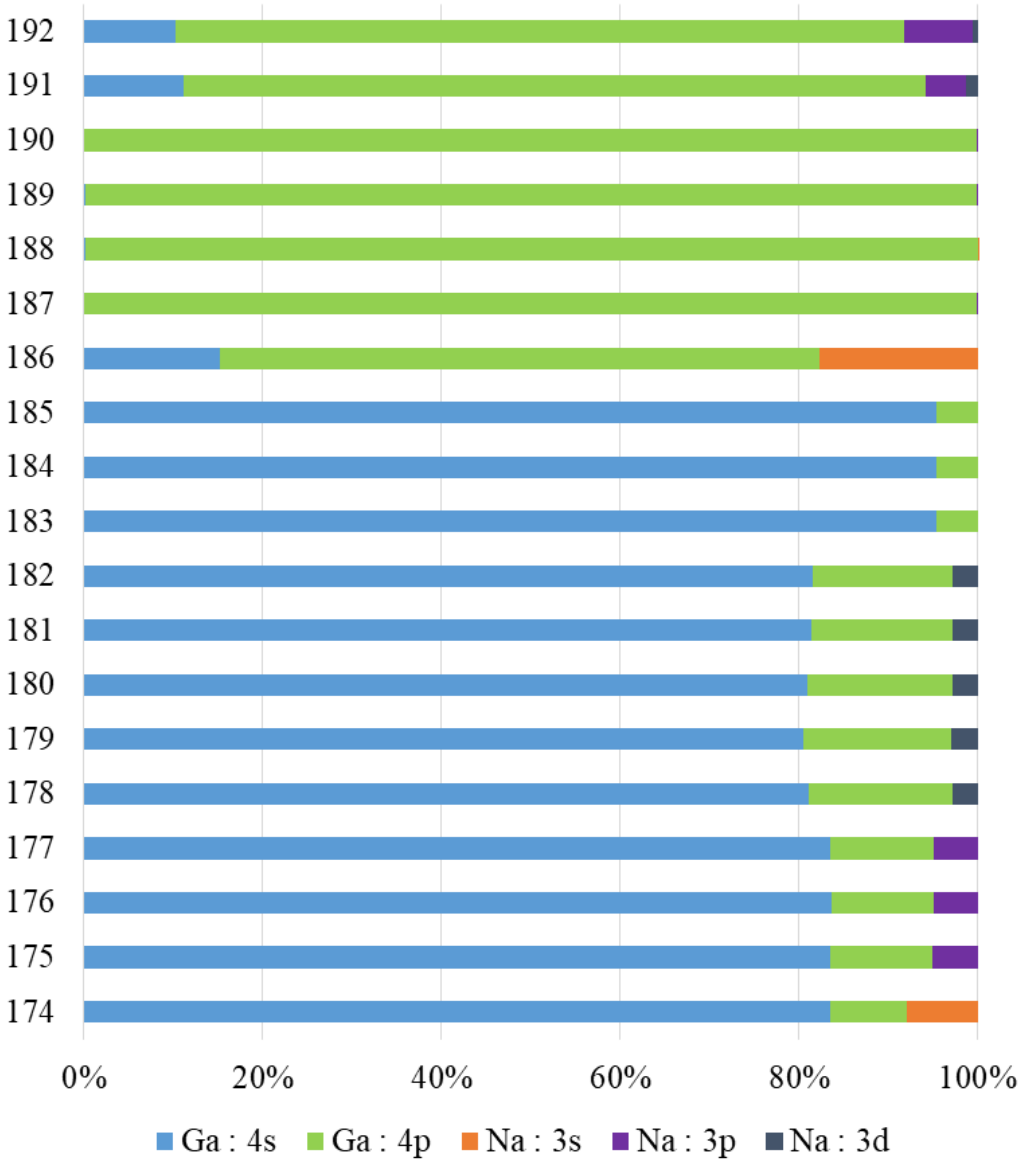

Figure S18. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Na@Ga_{12}$ cluster (interatomic Na-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

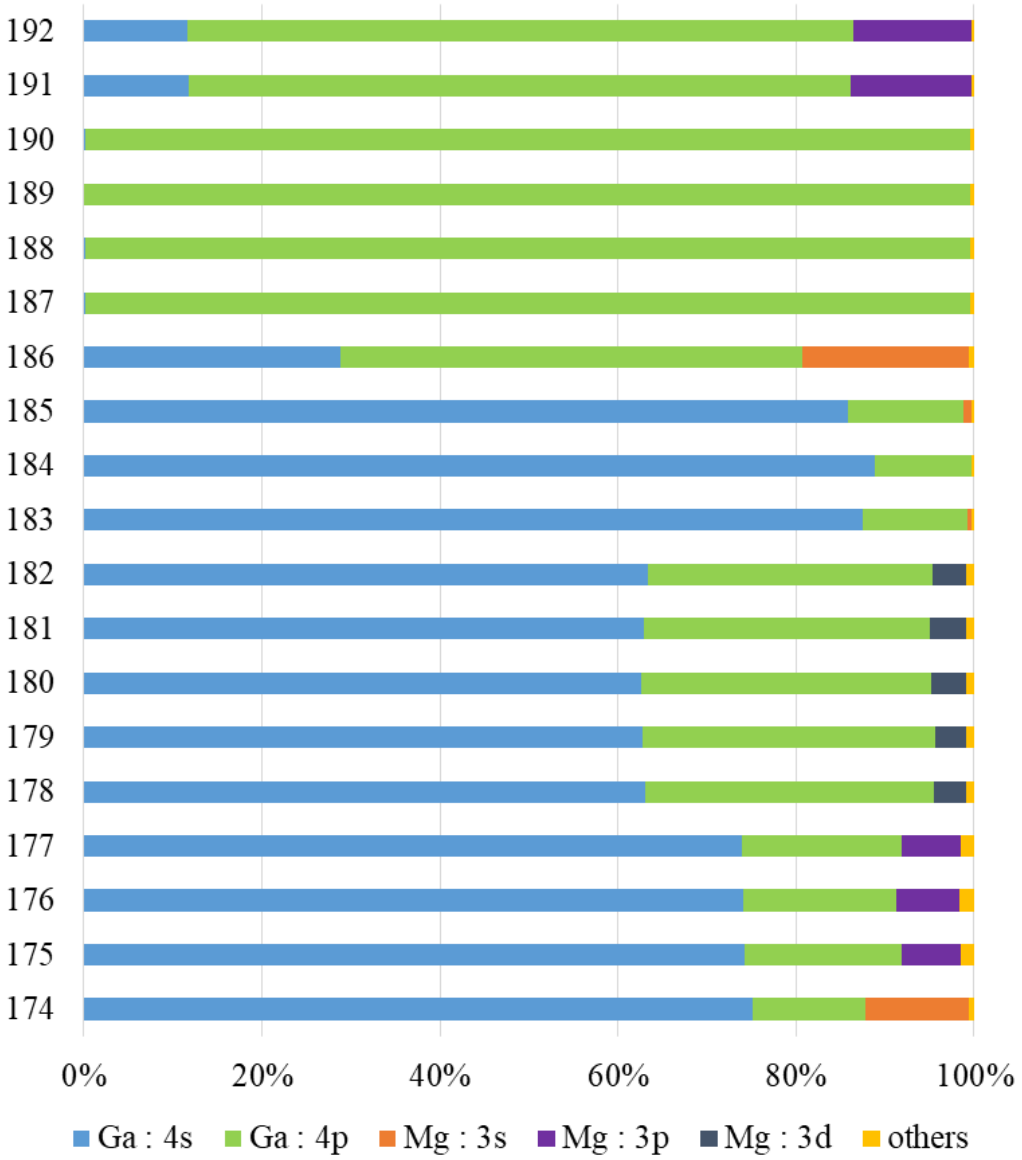

Figure S19. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Mg@Ga_{12}$ cluster (interatomic Mg-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis

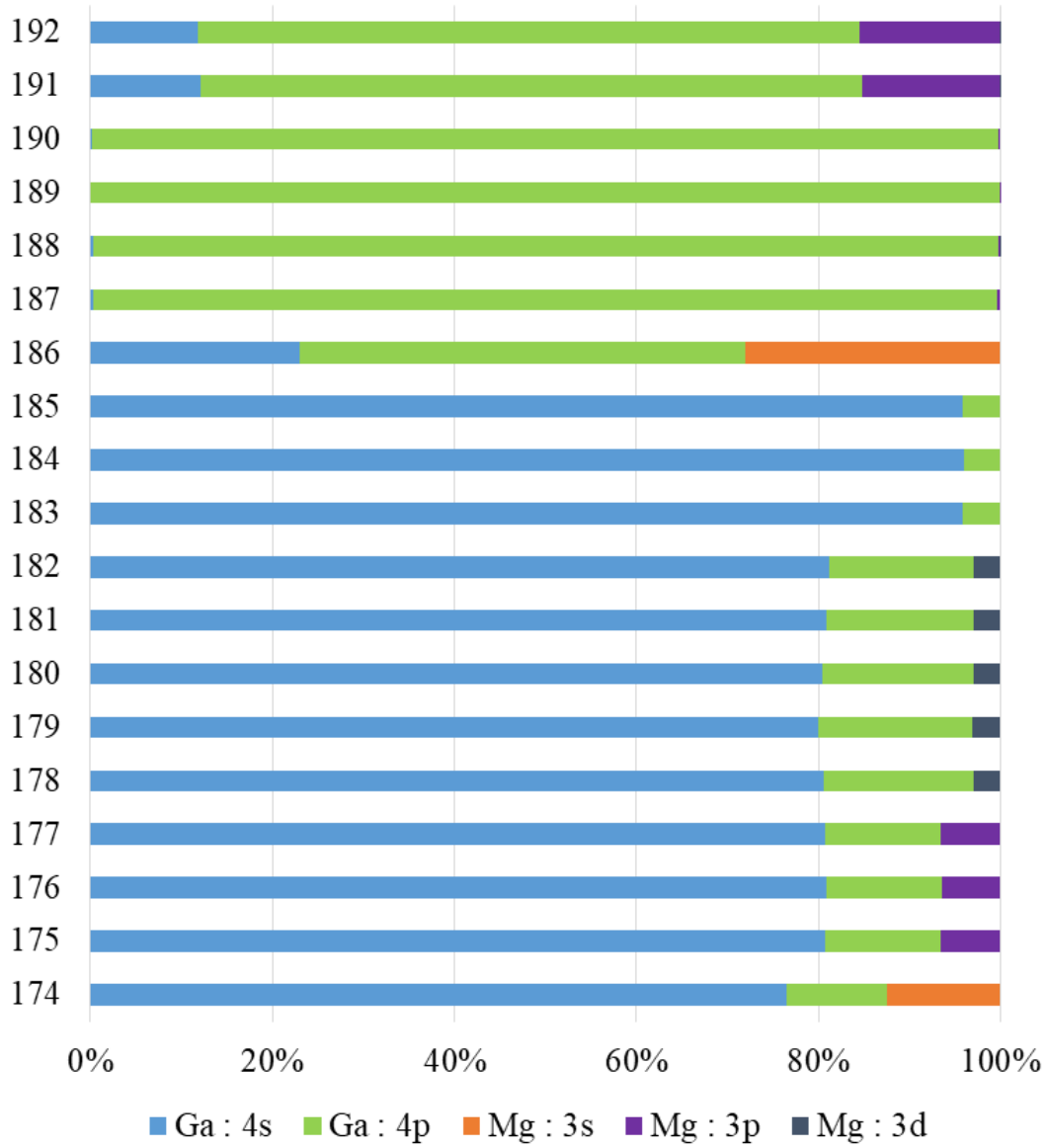

Figure S20. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Mg@Ga_{12}$ cluster (interatomic Mg-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

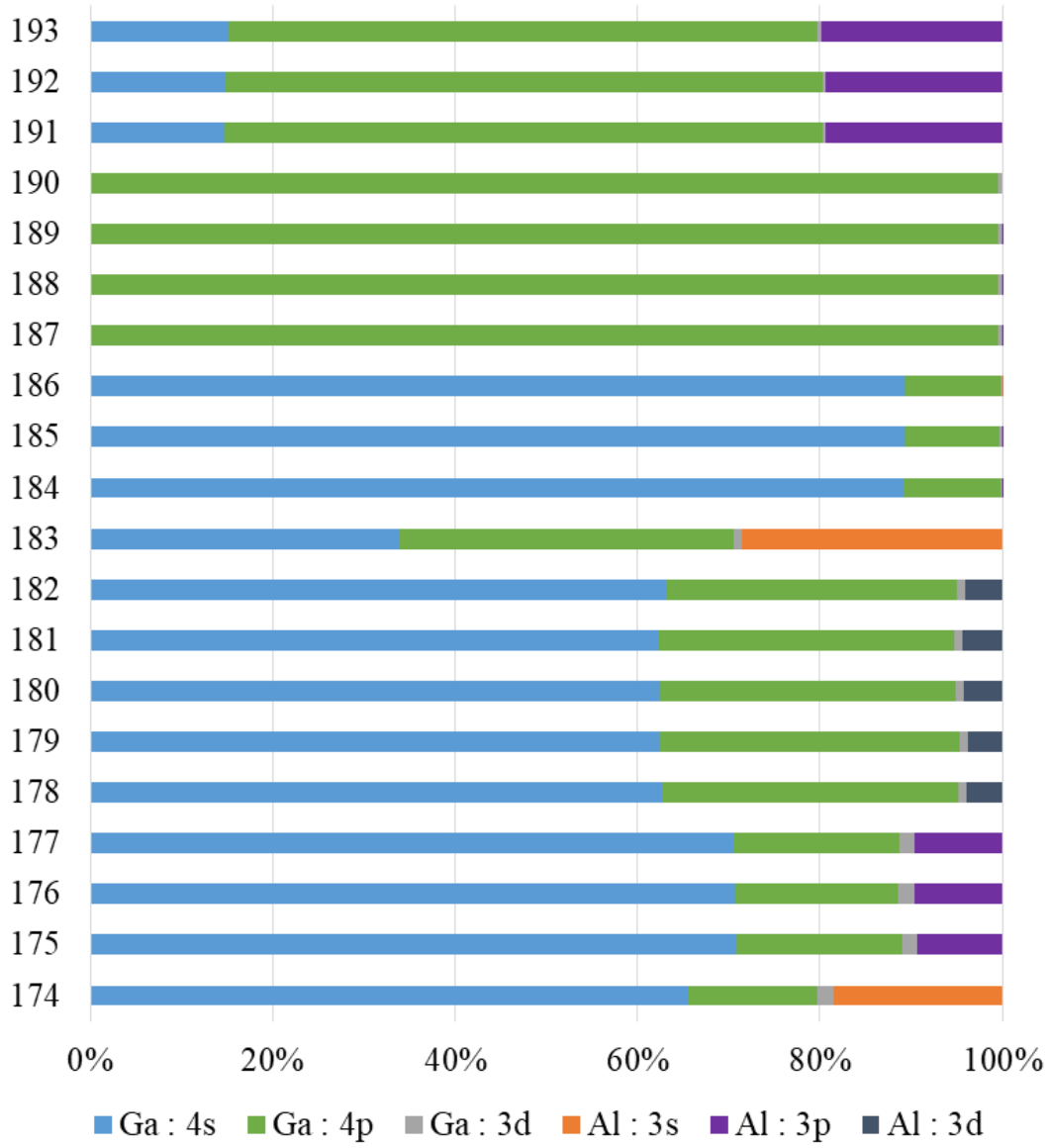

Figure S21. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the Al@Ga_{12} cluster (interatomic Al-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

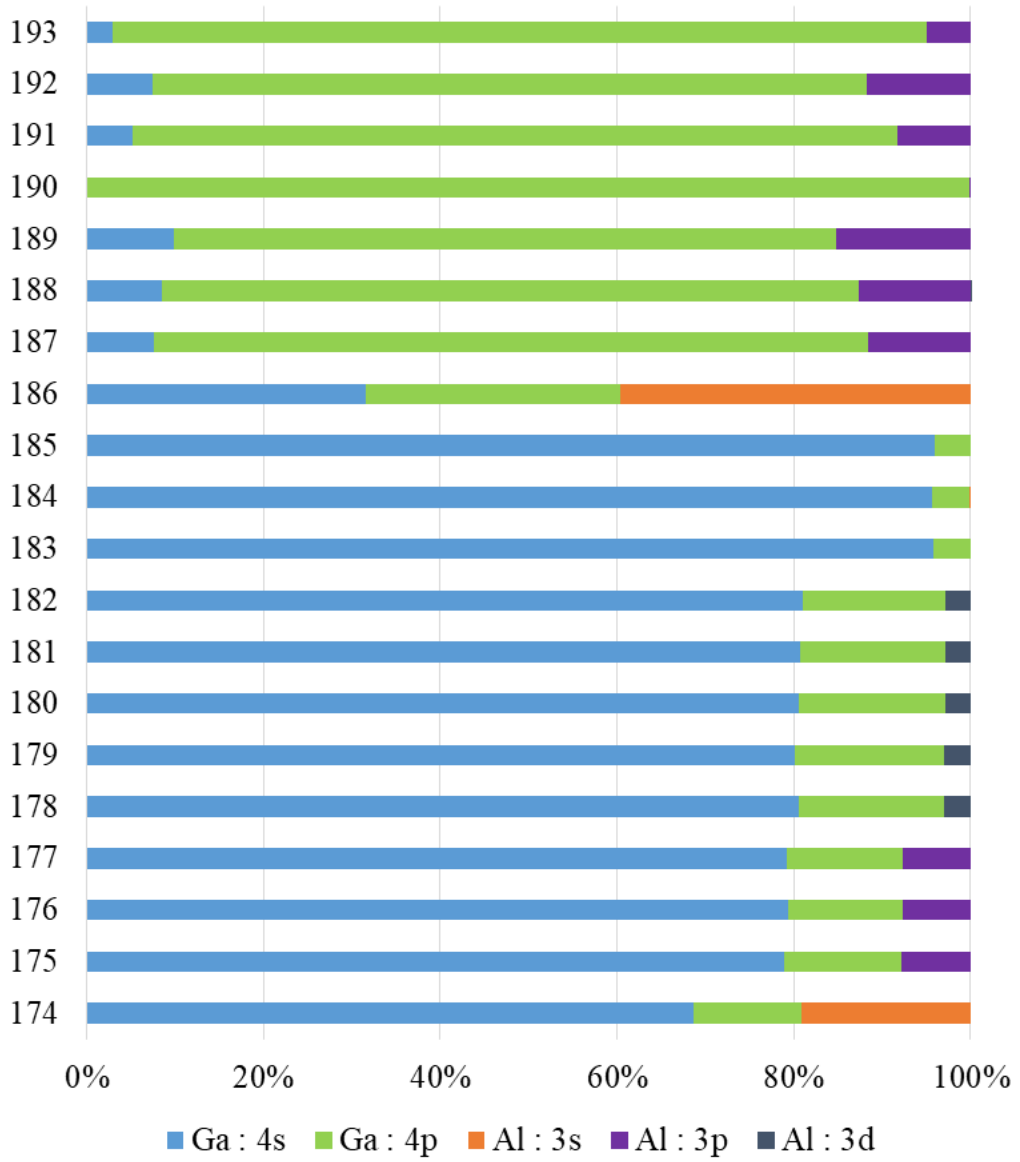

Figure S22. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Al@Ga_{12}$ cluster (interatomic Al-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

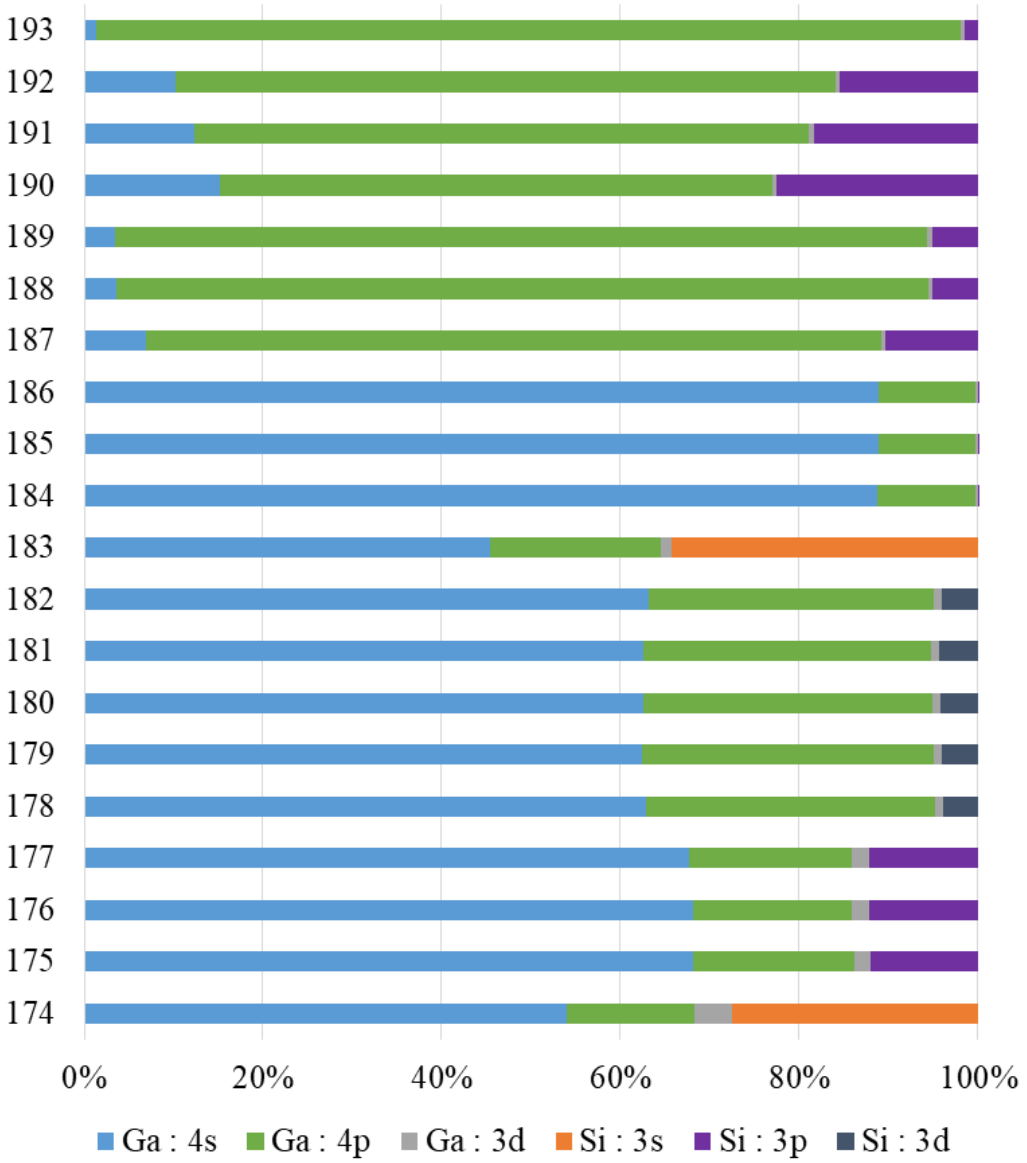

Figure S23. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Si@Ga_{12}$ cluster (interatomic Si-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

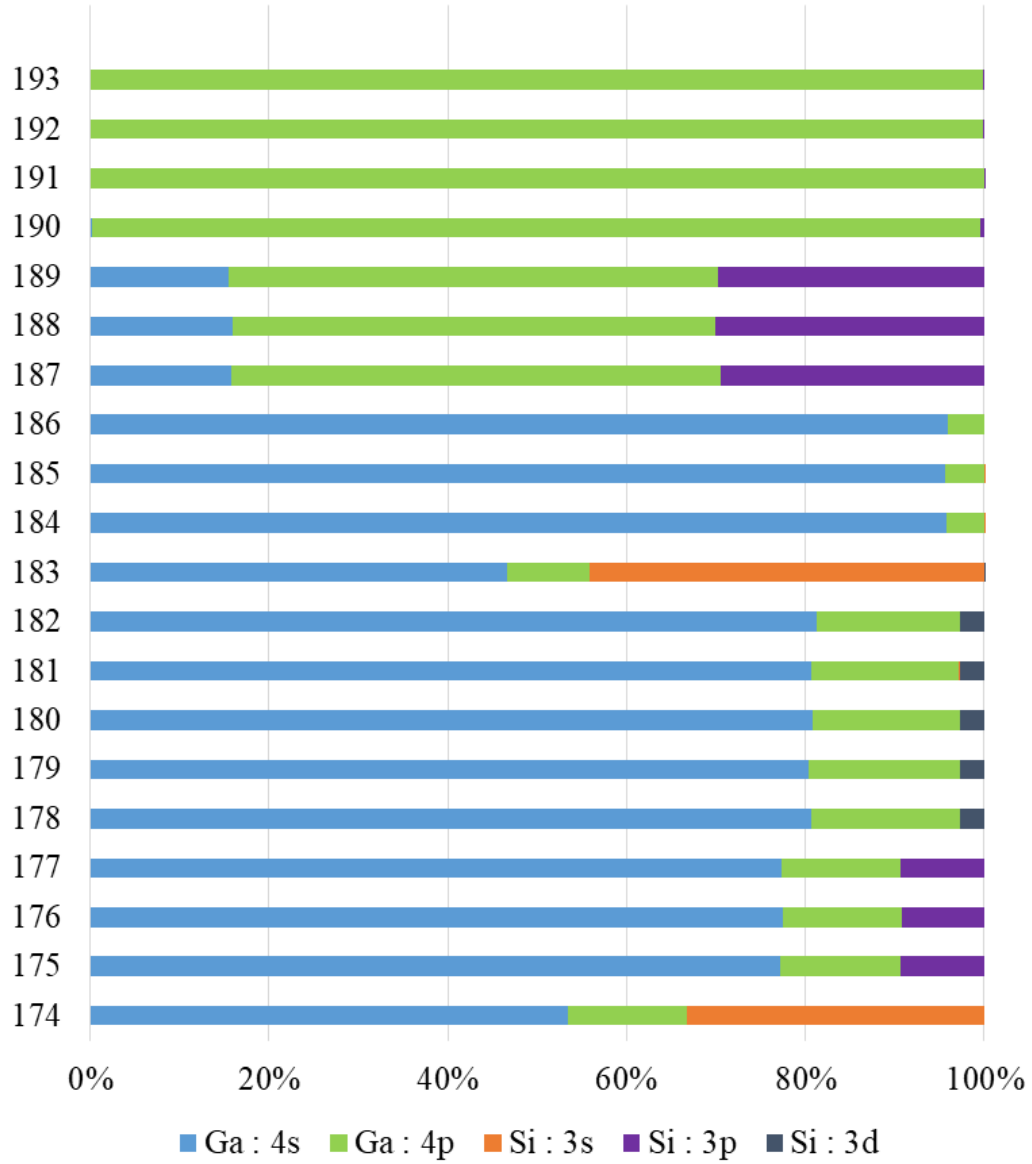

Figure S24. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Si@Ga_{12}$ cluster (interatomic Si-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

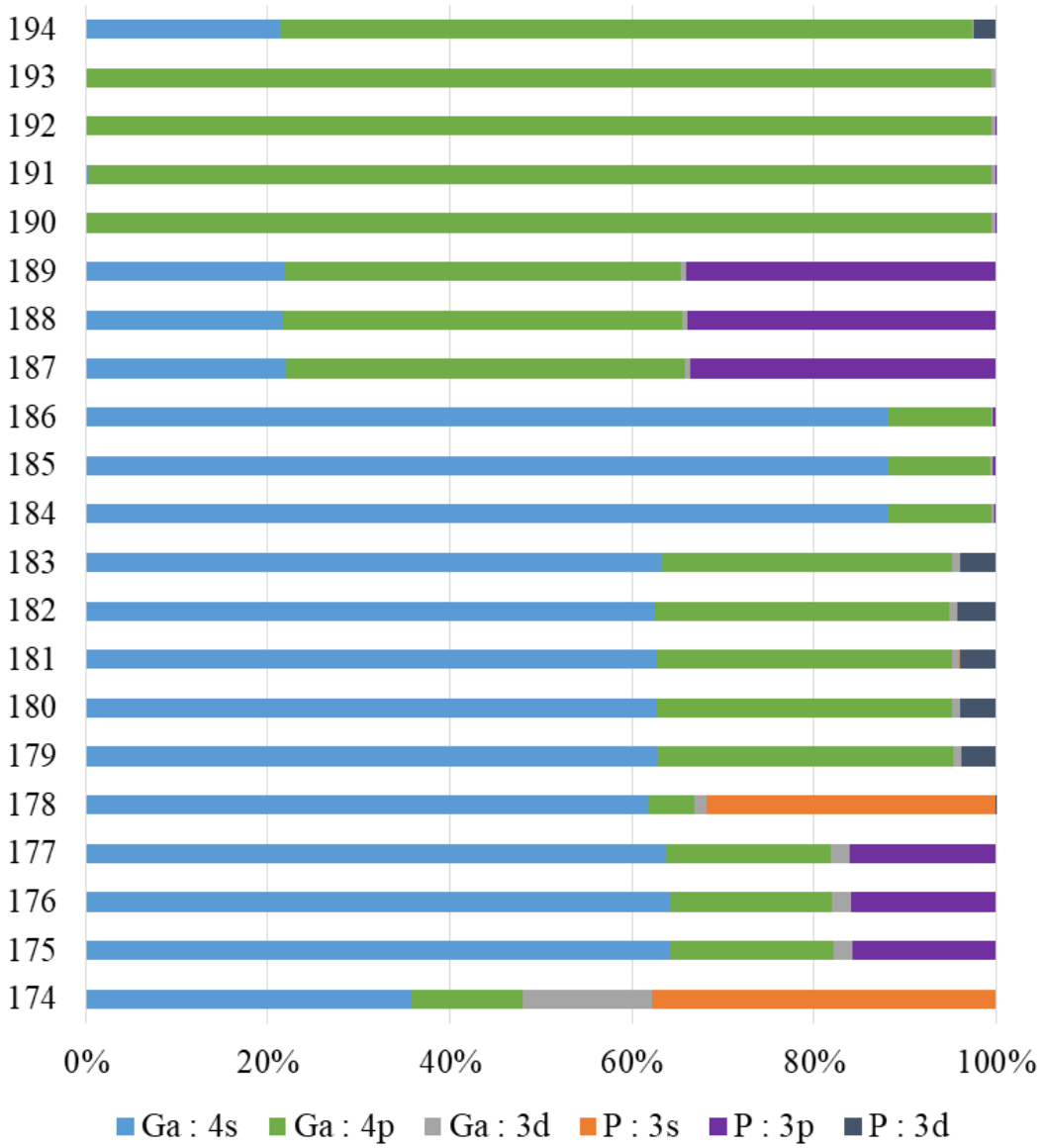

Figure S25. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the P@Ga_{12} cluster (interatomic P-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

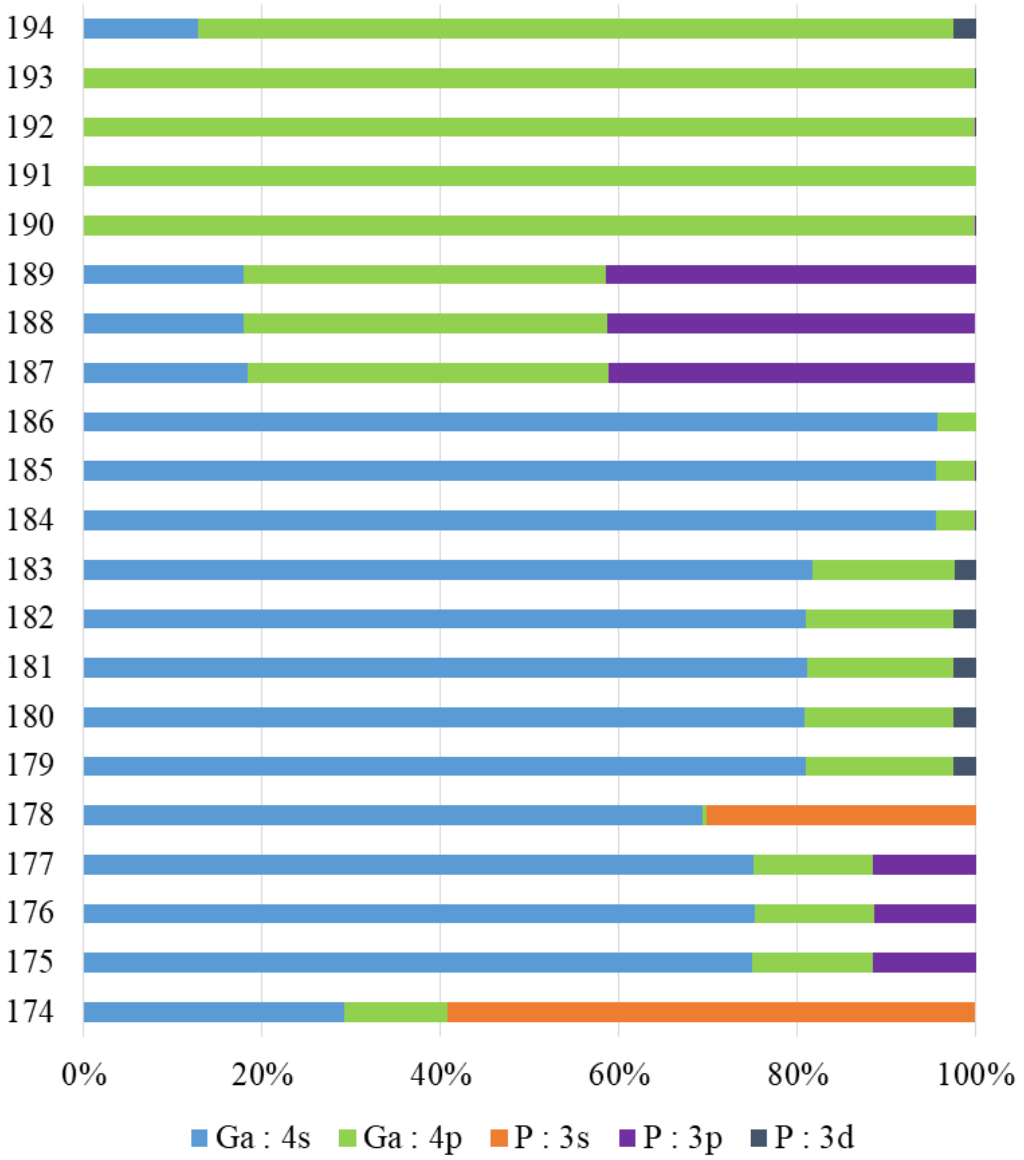

Figure S26. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the P@Ga_{12} cluster (interatomic P-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

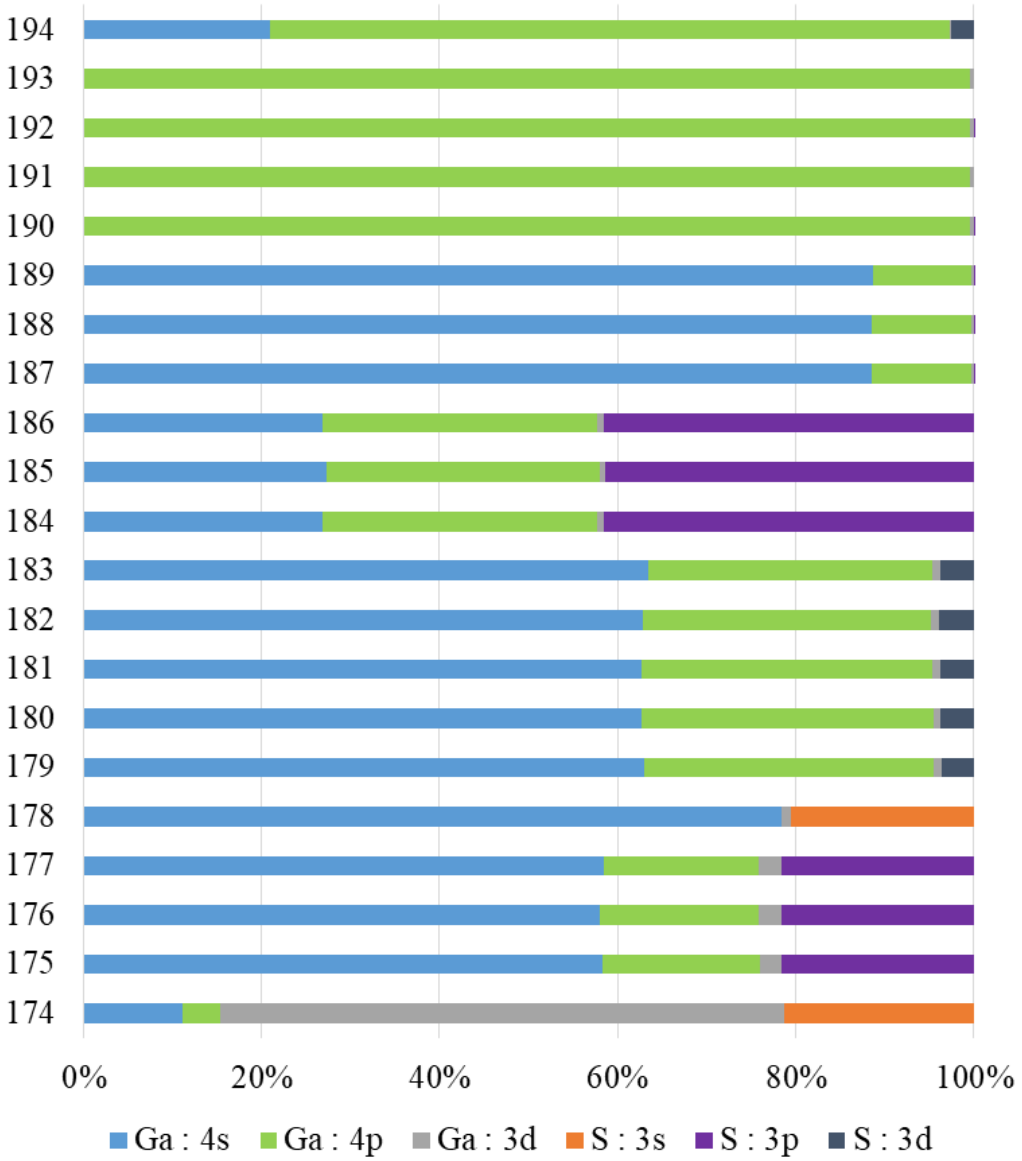

Figure S27. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the S@Ga_{12} cluster (interatomic S-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

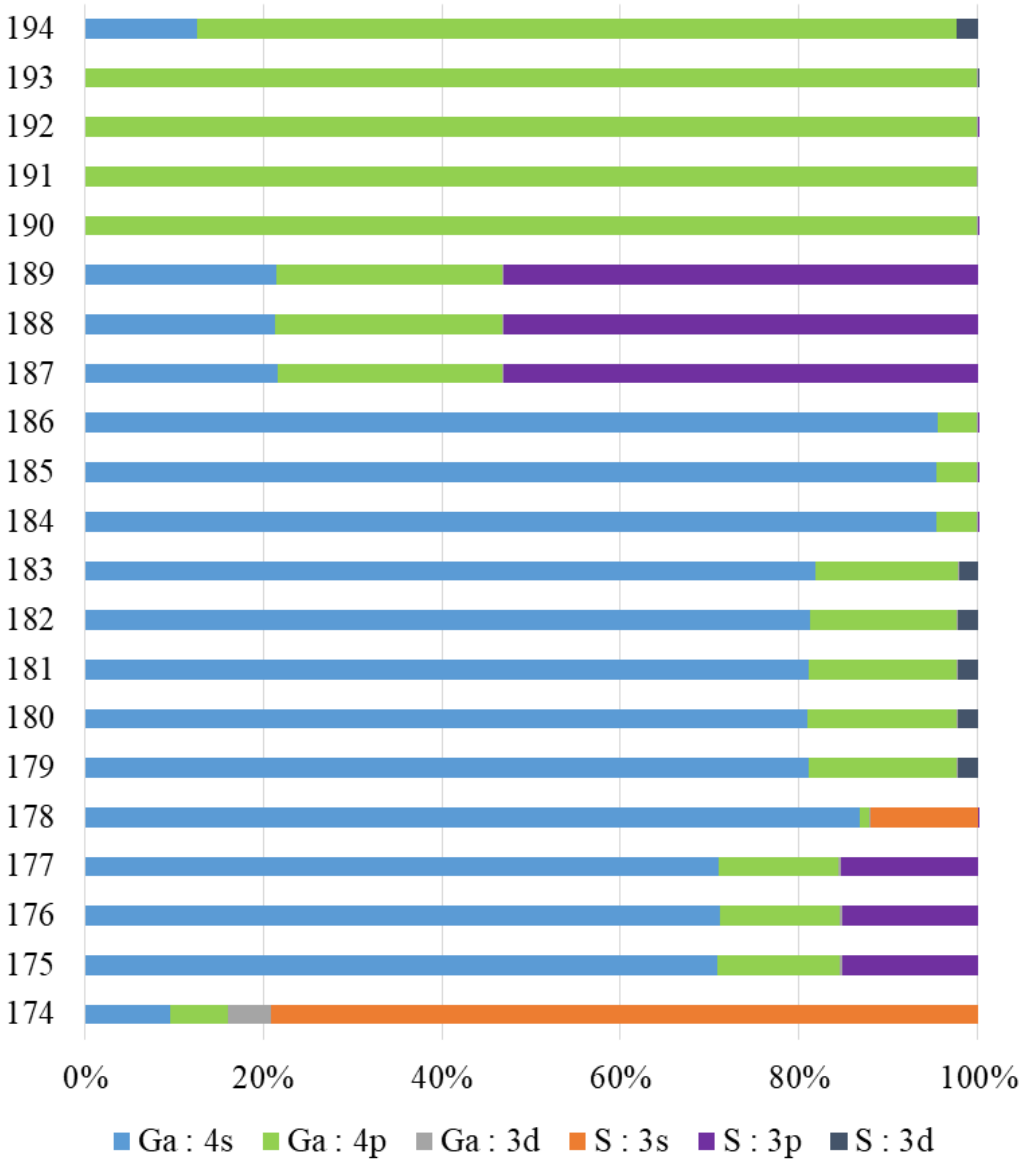

Figure S28. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the S@Ga_{12} cluster (interatomic S-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

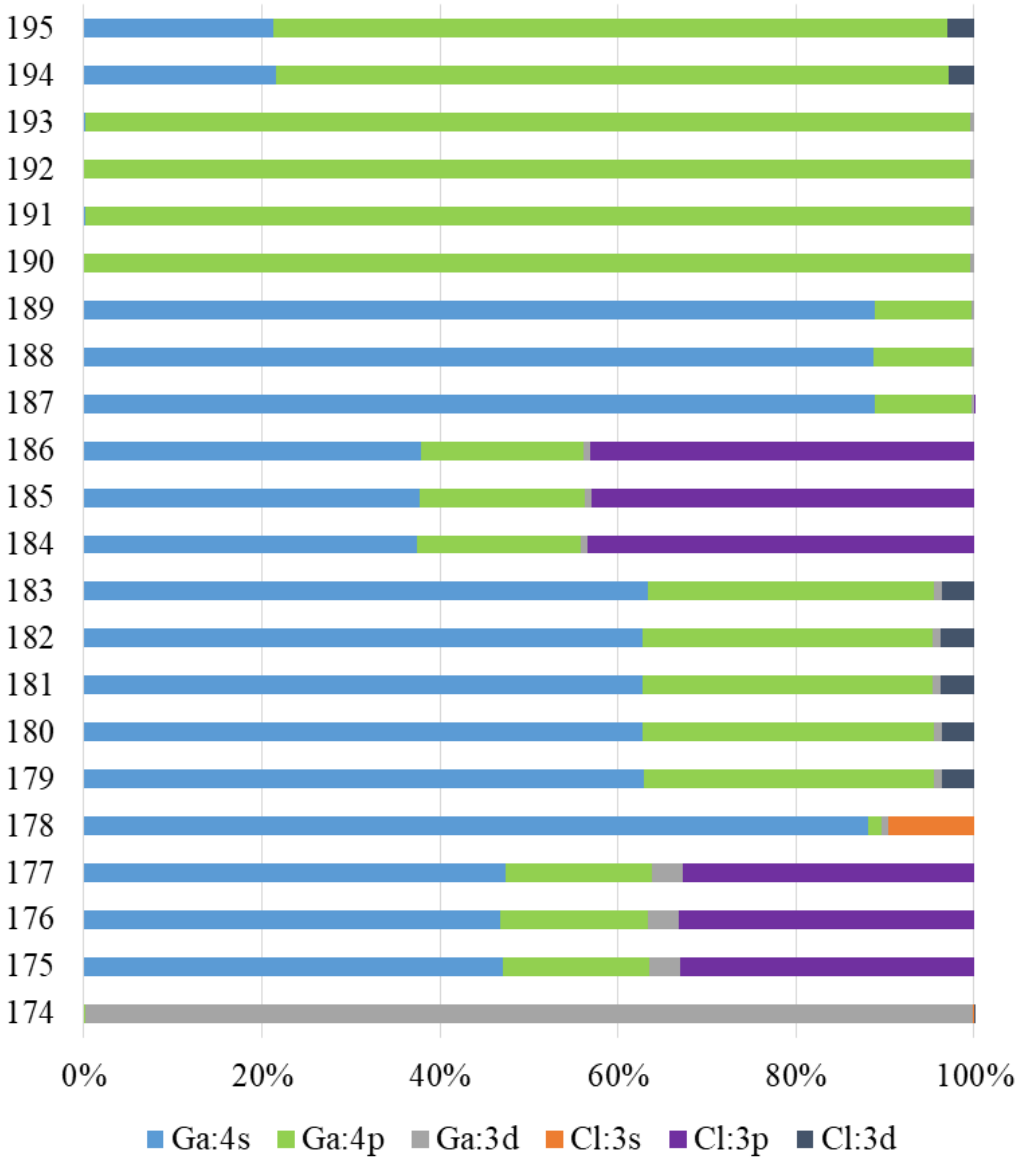

Figure S29. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the Cl@Ga_{12} cluster (interatomic Cl-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

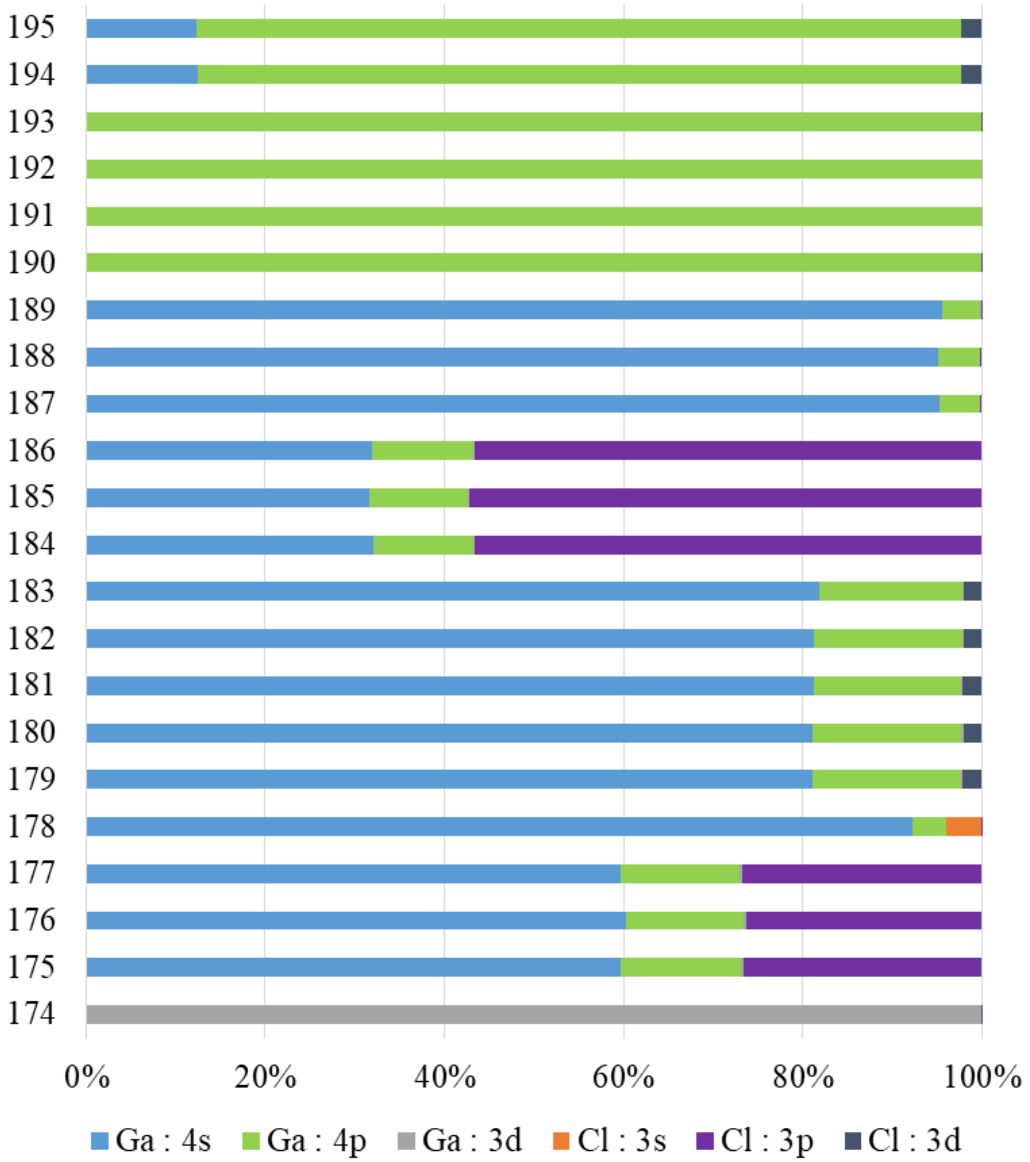

Figure S30. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the Cl@Ga_{12} cluster (interatomic Cl-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

Figure S31. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Ar@Ga_{12}$ cluster (interatomic Ar-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

Figure S32. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Ar@Ga_{12}$ cluster (interatomic Ar-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

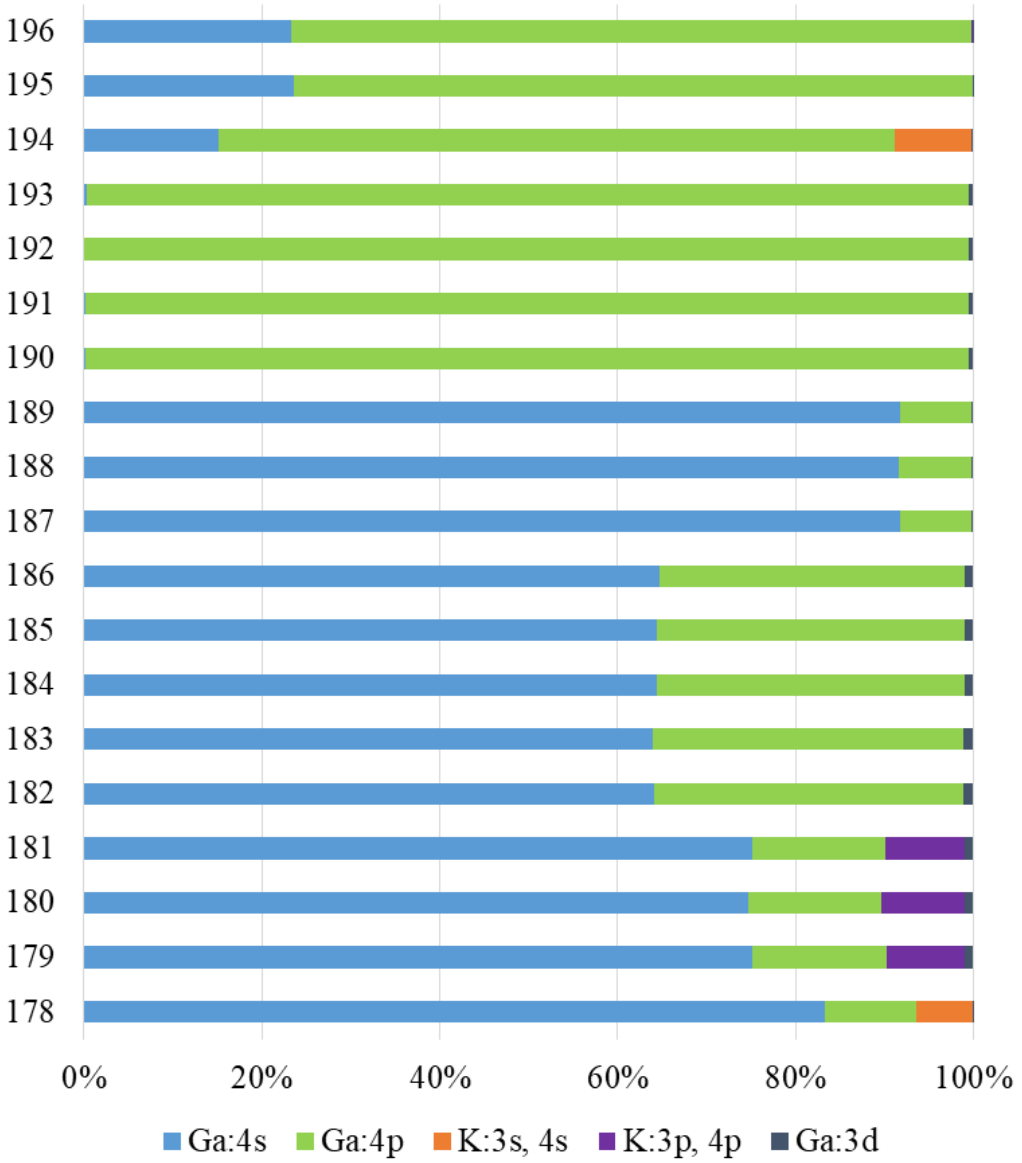

Figure S33. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the K@Ga_{12} cluster (interatomic K-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

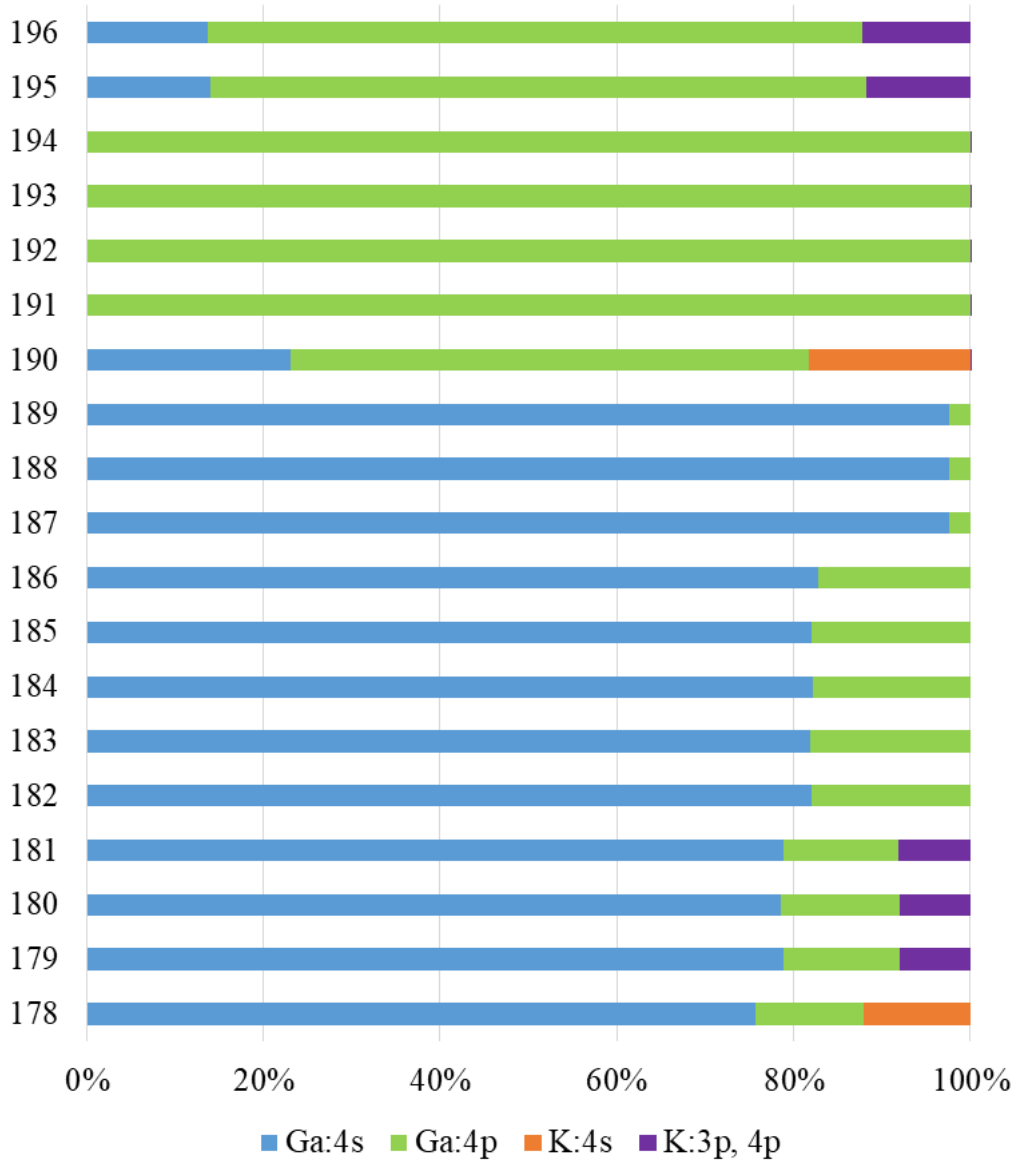

Figure S34. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the K@Ga_{12} cluster (interatomic K-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

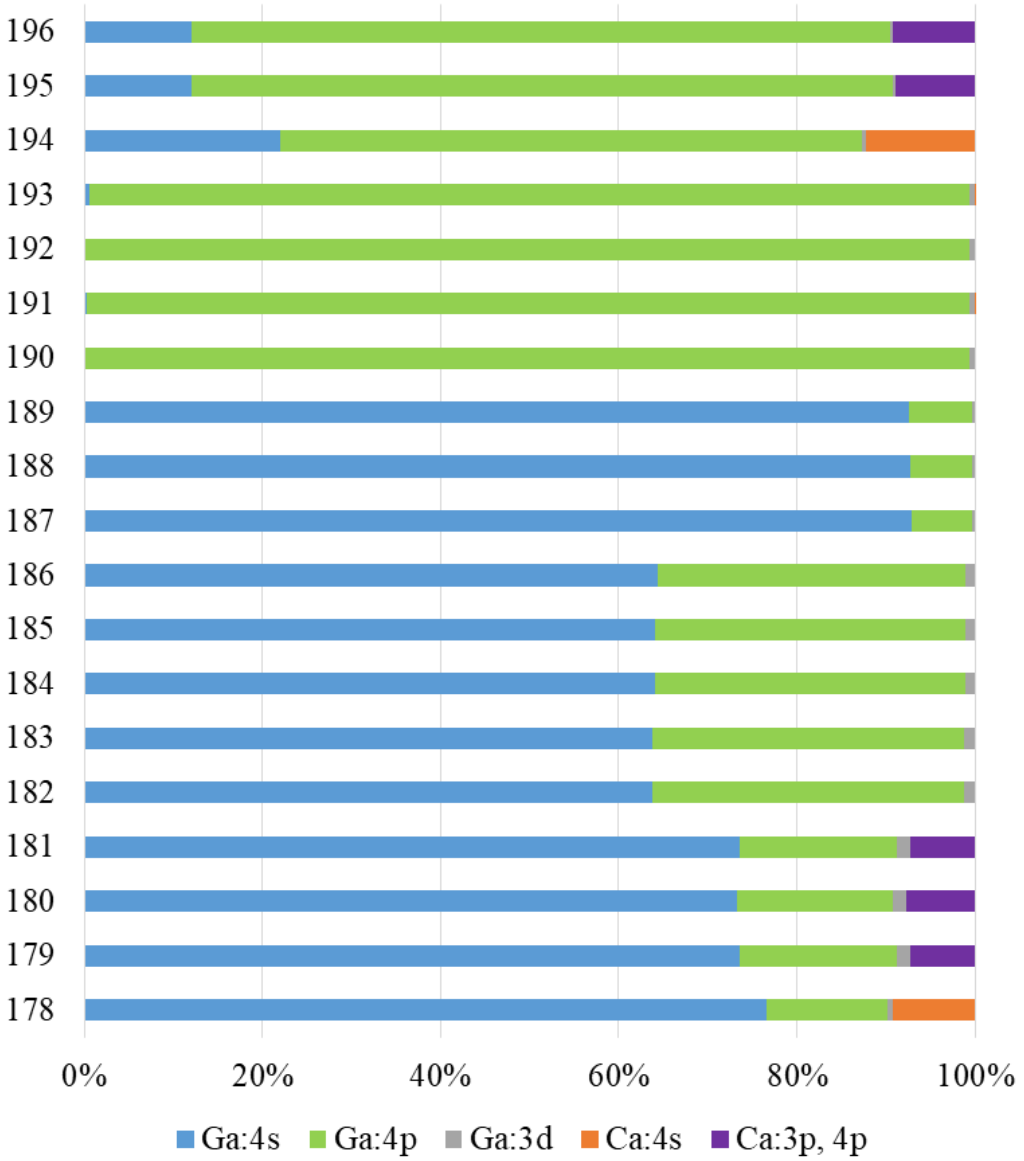

Figure S35. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Ca@Ga_{12}$ cluster (interatomic Ca-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

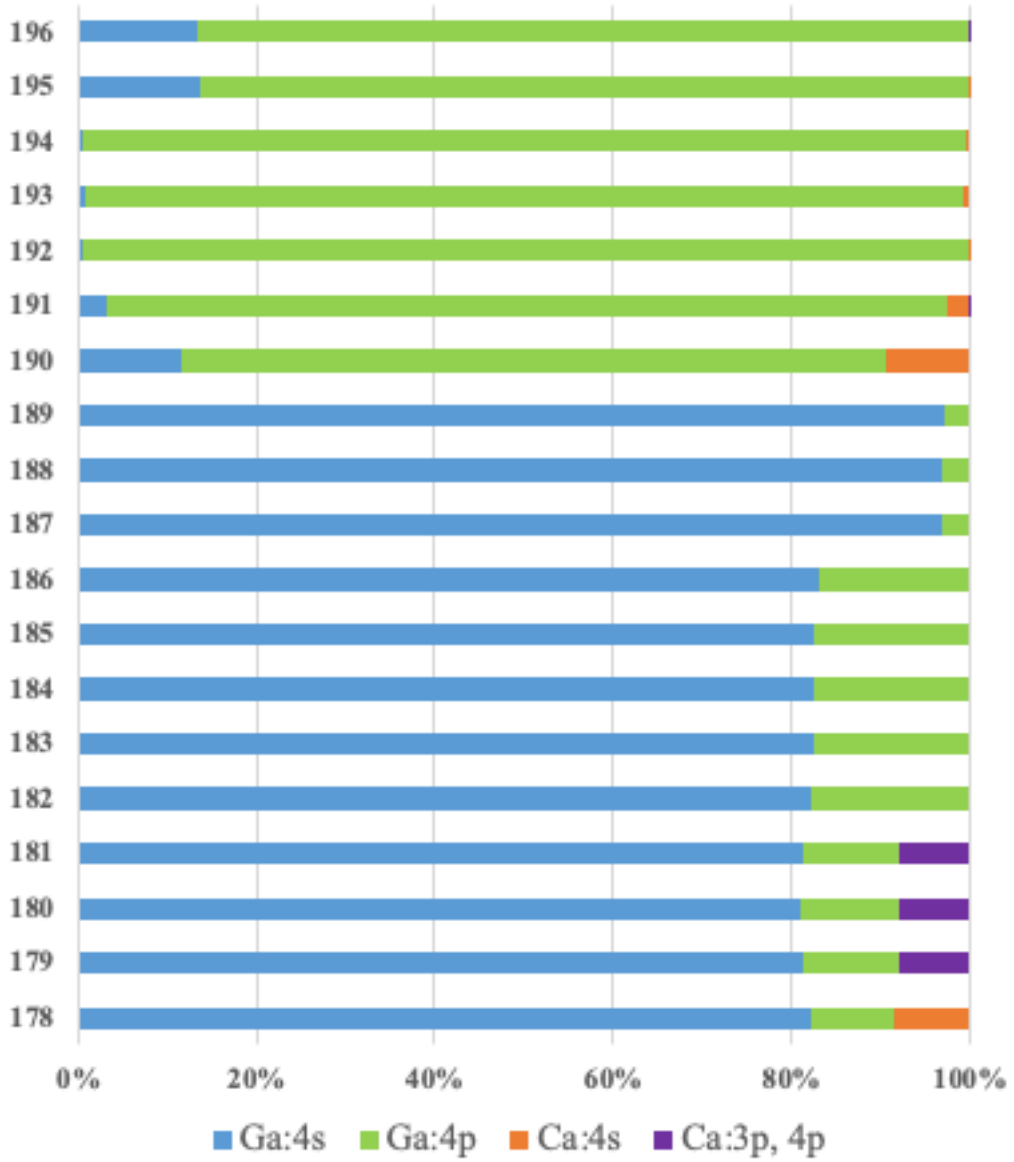

Figure S36. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Ca@Ga_{12}$ cluster (interatomic Ca-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

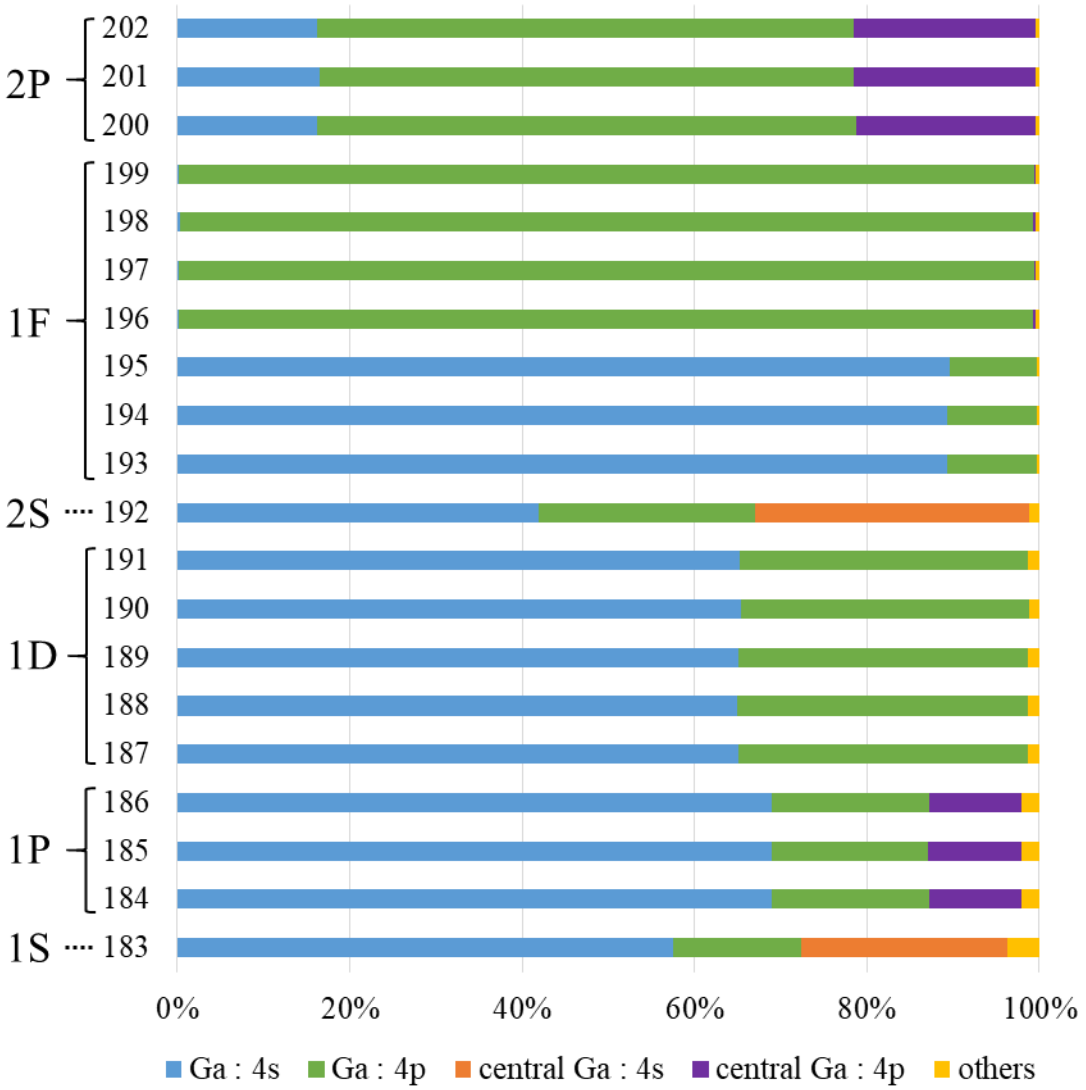

Figure S37. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Ga@Ga_{12}$ (Ga_{13}) cluster (interatomic Ga-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis. (***Figure 8***)

Figure S38. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Ga@Ga_{12}$ (Ga_{13}) cluster (interatomic Ga-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

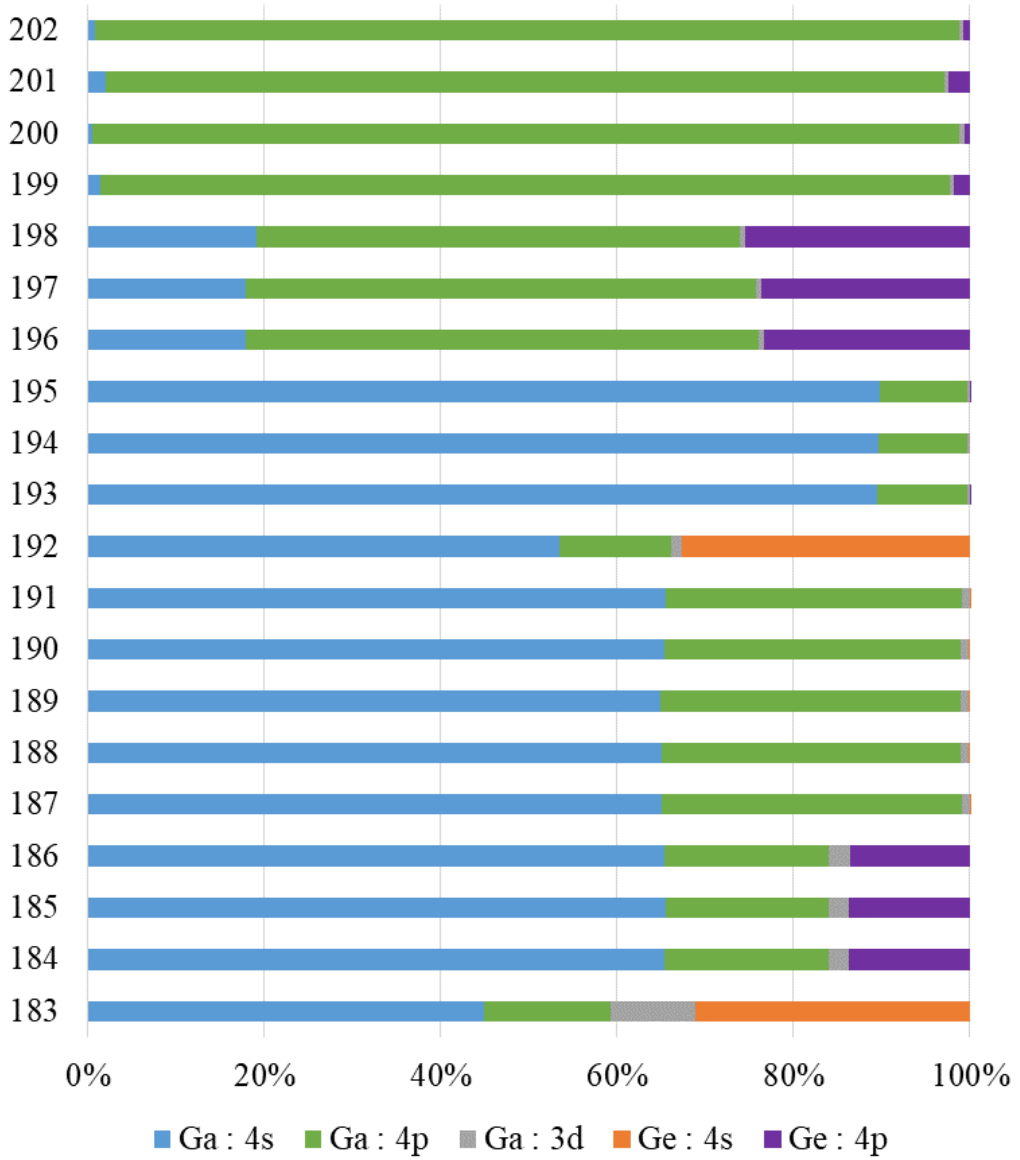

Figure S39. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the Ge@Ga_{12} cluster (interatomic Ge-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

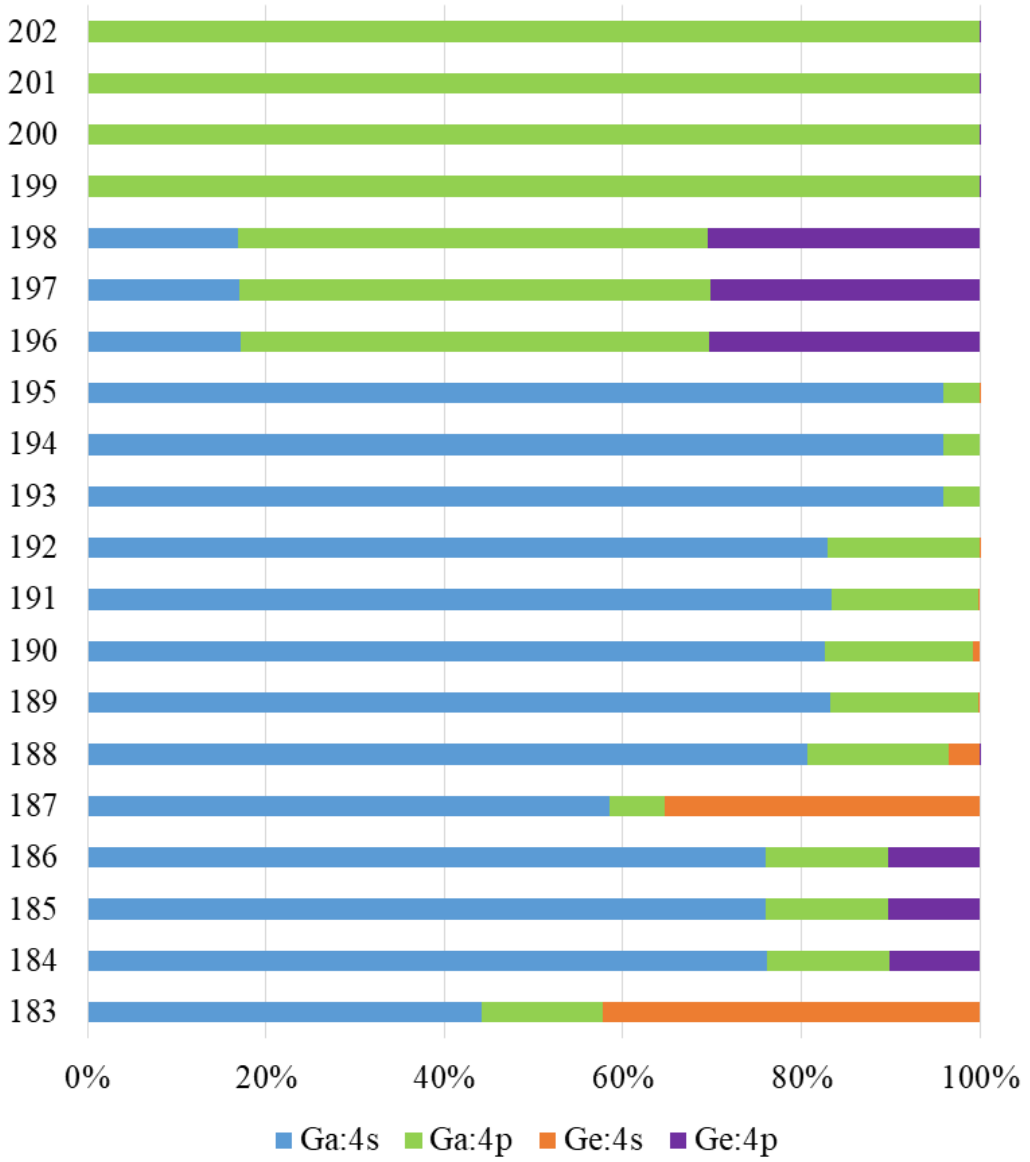

Figure S40. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the Ge@Ga_{12} cluster (interatomic Ge-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

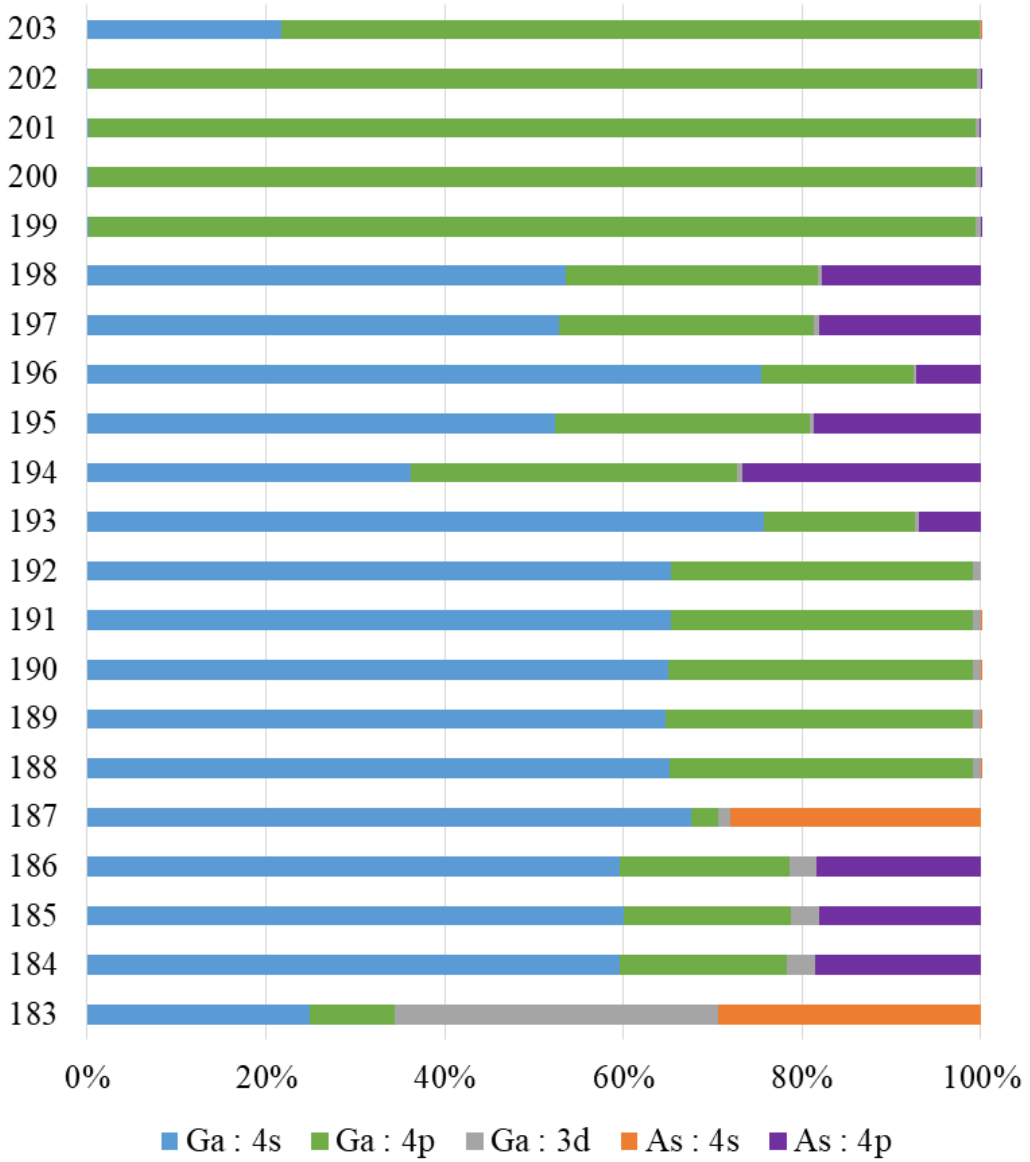

Figure S41. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the As@Ga_{12} cluster (interatomic As-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis. (***Figure13***)

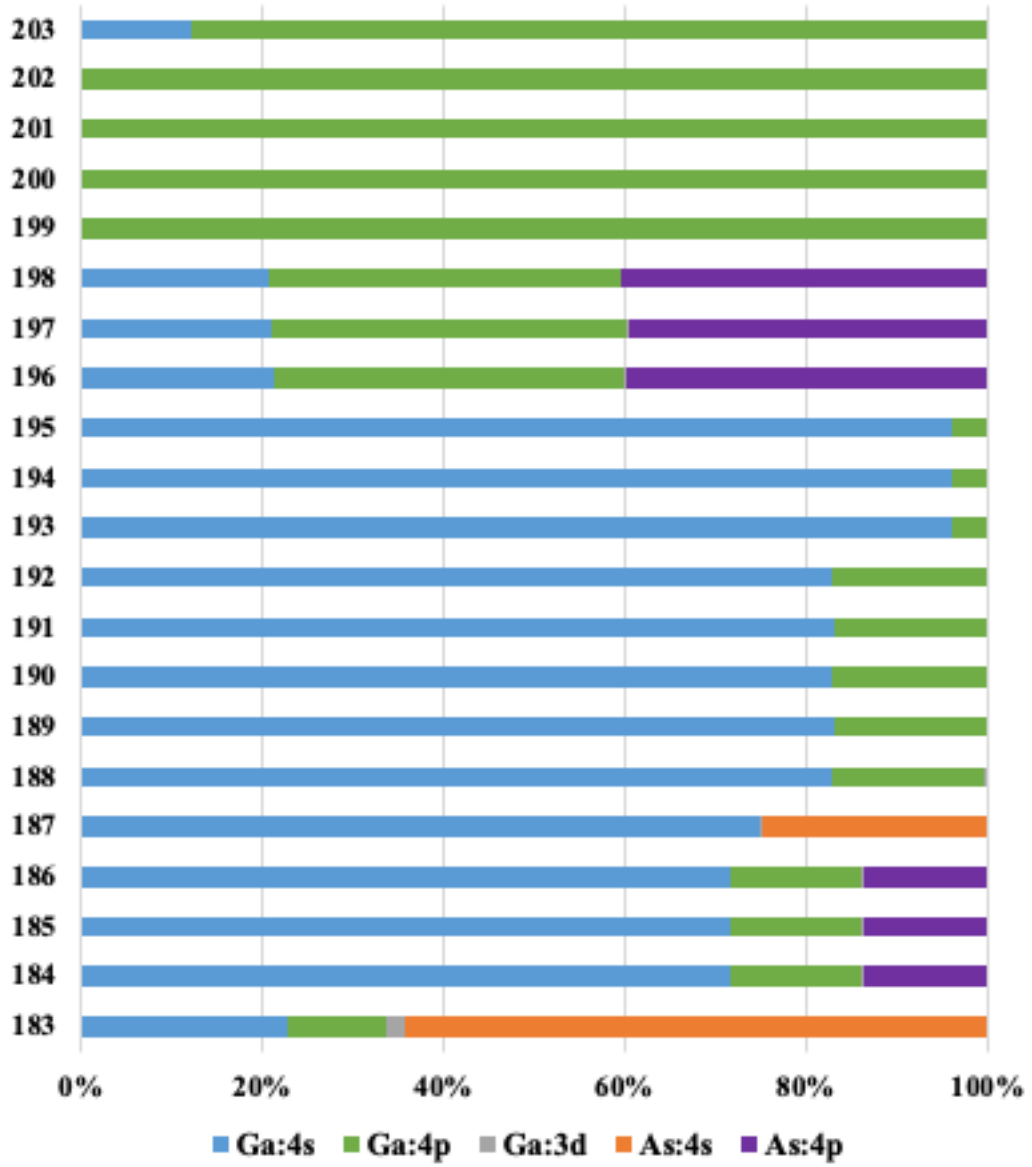

Figure S42. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the As@Ga_{12} cluster (interatomic As-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

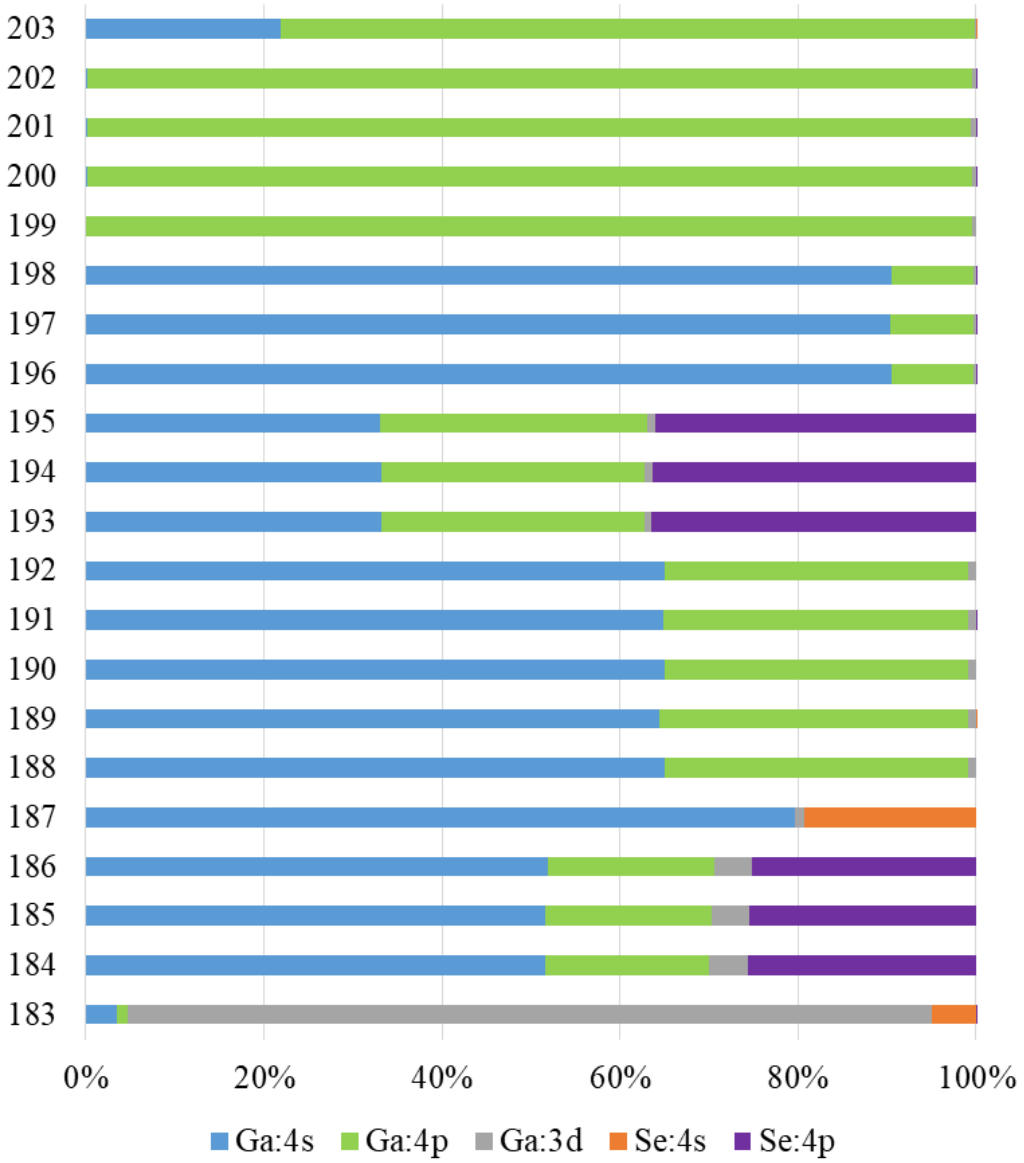

Figure S43. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the Se@Ga_{12} cluster (interatomic Se-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

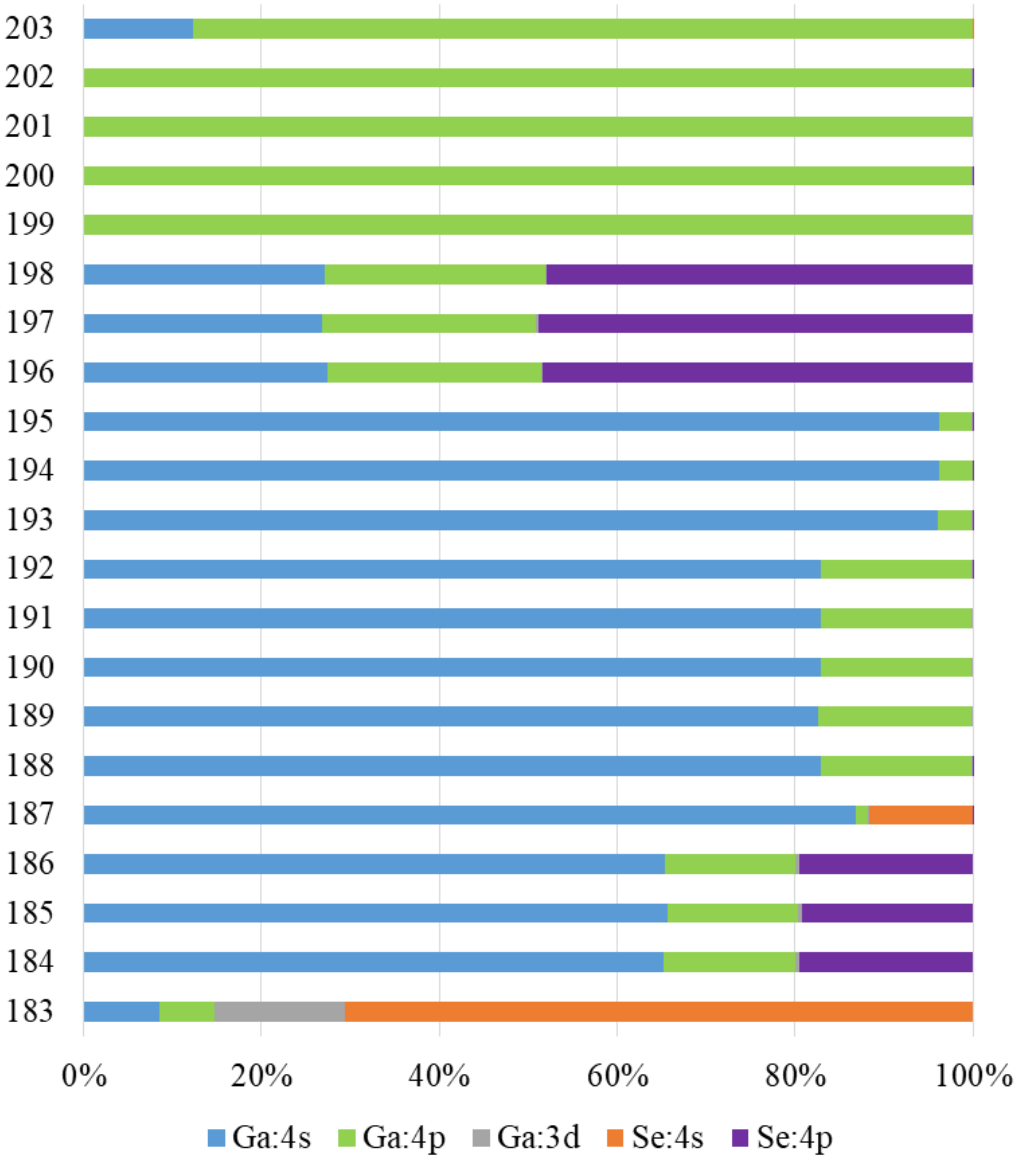

Figure S44. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the Se@Ga_{12} cluster (interatomic Se-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

Figure S45. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the Br@Ga_{12} cluster (interatomic Br-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

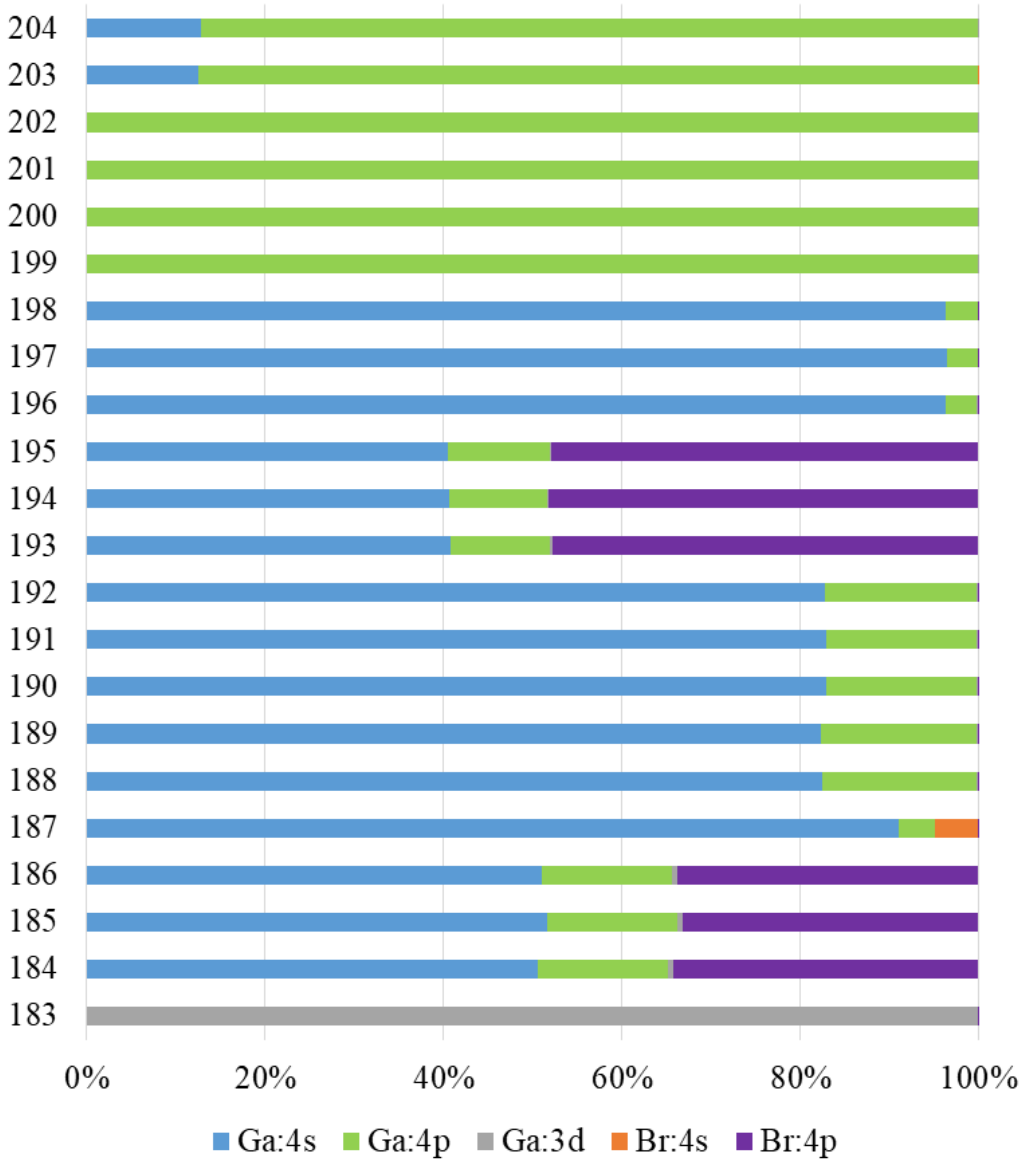

Figure S46. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the Br@Ga_{12} cluster (interatomic Br-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.

Figure S47. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Kr@Ga_{12}$ cluster (interatomic Kr-Ga bond distance is 2.547 Å) by means of the Mulliken population analysis.

Figure S48. Ratio of atomic orbitals in order to create the superatomic-like orbitals of the $Kr@Ga_{12}$ cluster (interatomic Kr-Ga bond distance is 2.944 Å) by means of the Mulliken population analysis.