



**Fig. S1** Plots of orbital energy levels (eV) and dominant excitations for 1-component (SF) a)  $\text{Ag}_3^+$ , b)  $\text{Au}_3^+$ , c)  $\text{Ag}_2\text{Au}^+$ , d)  $\text{AgAu}_2^+$ , and 2-component (SO) e)  $\text{Ag}_3^+$ , f)  $\text{Au}_3^+$ , g)  $\text{Ag}_2\text{Au}^+$ , h)  $\text{AgAu}_2^+$  along with the color-coded s-character and Ag/Au-character (in c, d) for each orbital. Only the strongest excitation for each visible peak is shown together with the corresponding transition dipole moment operator. Thickness of each arrow branch is in proportion to the orbital contribution to the excitation (orbitals contributing less than 10% are neglected).