

Fig. S1 The contour plots of $\nabla^2\rho_{\text{BCP}}$ for the triel-bonded complexes. Green solid lines represent the region of $\nabla^2\rho_{\text{BCP}} > 0$ and purple dashed lines highlight the area of $\nabla^2\rho_{\text{BCP}} < 0$

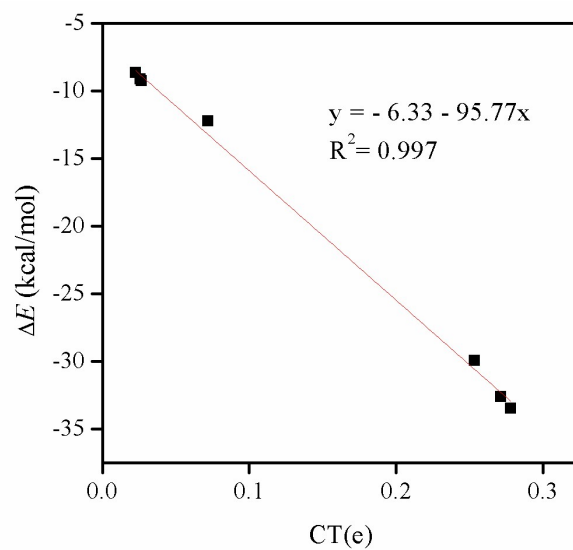


Fig. S2 Relationship between interaction energy (ΔE) and charge transfer (CT) in the chalcogen-bonded complexes

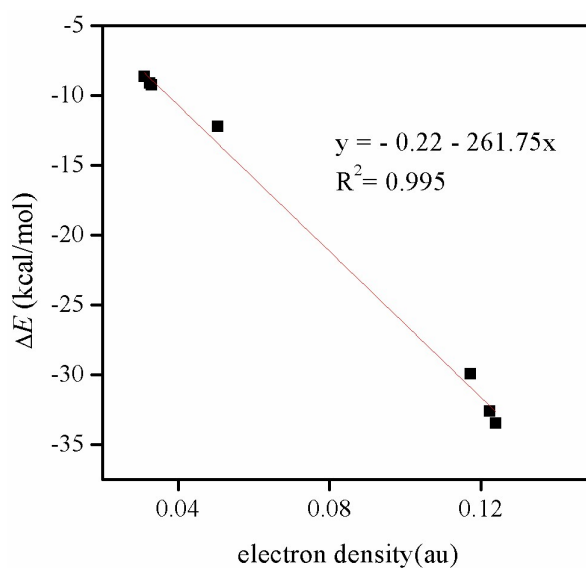


Fig. S3 Relationship between interaction energy (ΔE) and energy density in the chalcogen-bonded complexes

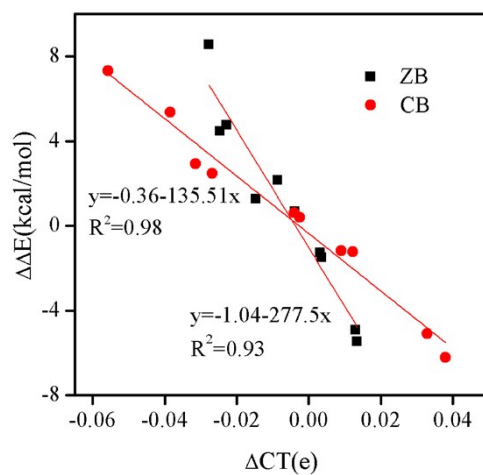


Fig. S4 Relationship between the change of interaction energy ($\Delta\Delta E$) and change of charge transfer (ΔCT) of triel bond (ZB) and chalcogen bond (CB) in the triads relative to the dyads