Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Gold(III) derivatives as the noncovalent interaction donors: theoretical study of the π-hole regium bonds

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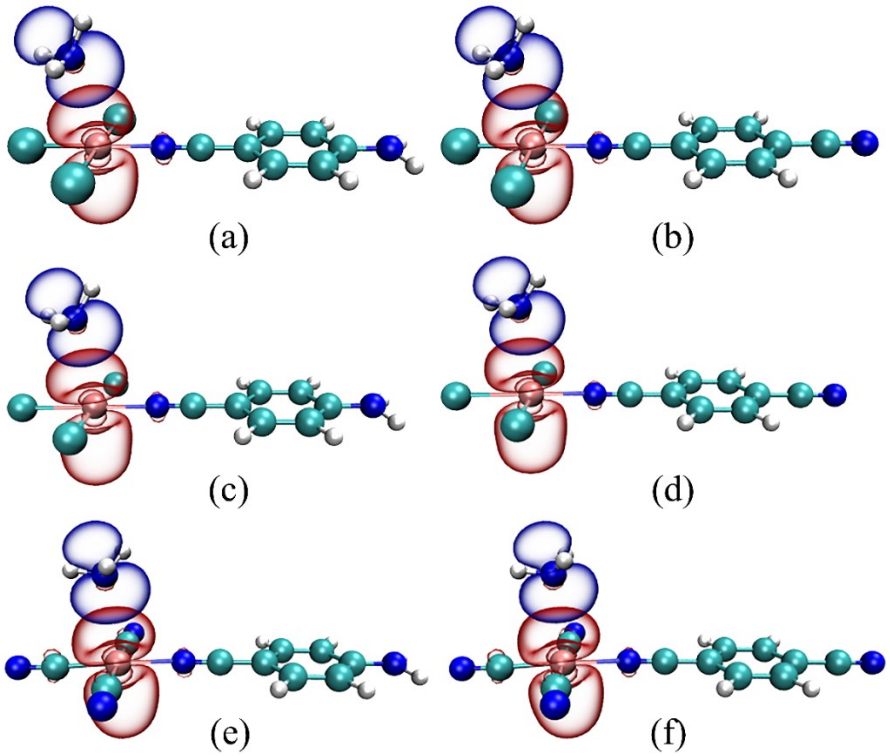

Fig. S1 Schematic diagrams of main orbital interactions. (a) **1**…NH_3; (b) **5**…NH_3; (c) **6**…NH_3; (d) **10**…NH_3; (e) **11**…NH_3; (f) **15**…NH_3.

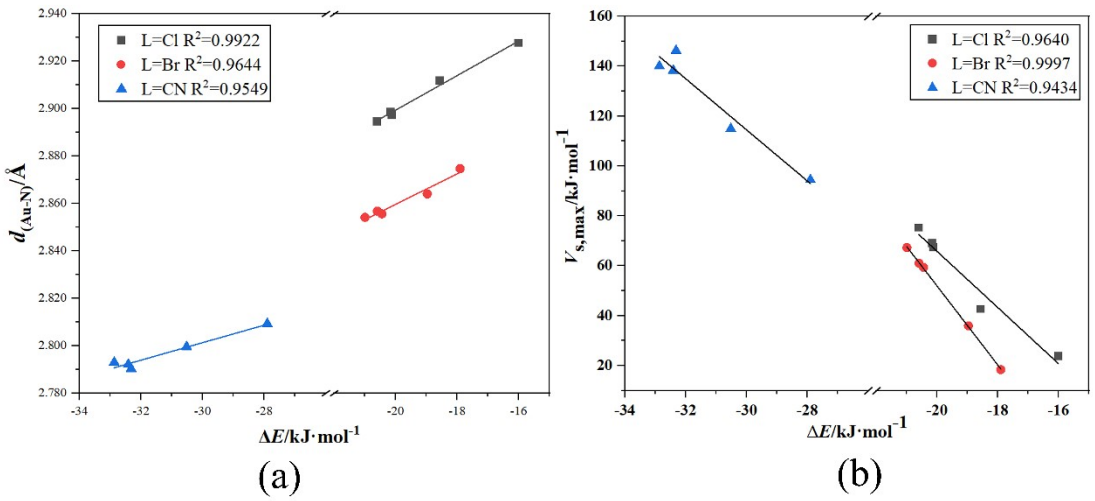

Fig. S2 (a) Correlation between the binding energy (ΔE) and the binding distance ($d_{(Au\cdots N)}$); (b) correlation between the binding energy (ΔE) and the MEP value over the Au atom ($V_{s,max(Au)}$).

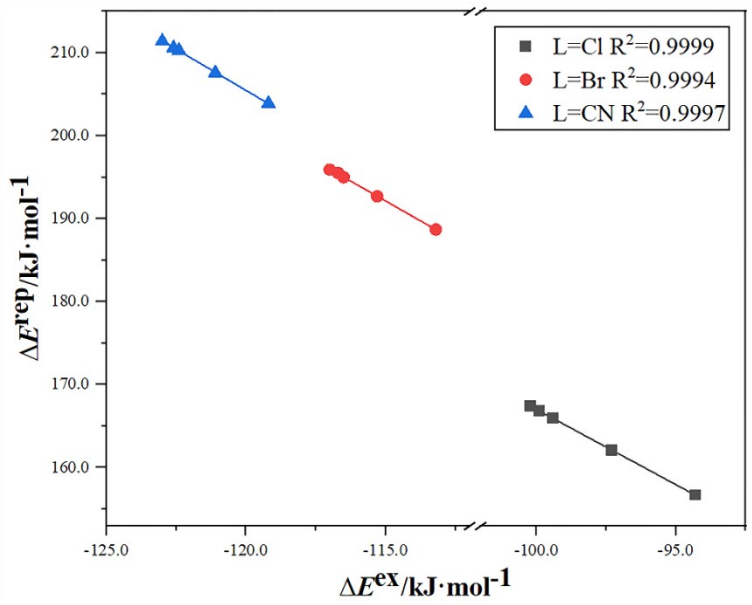

Fig. S3 Correlation between exchange energy (ΔE^{ex}) and repulsion energy (ΔE^{rep}).

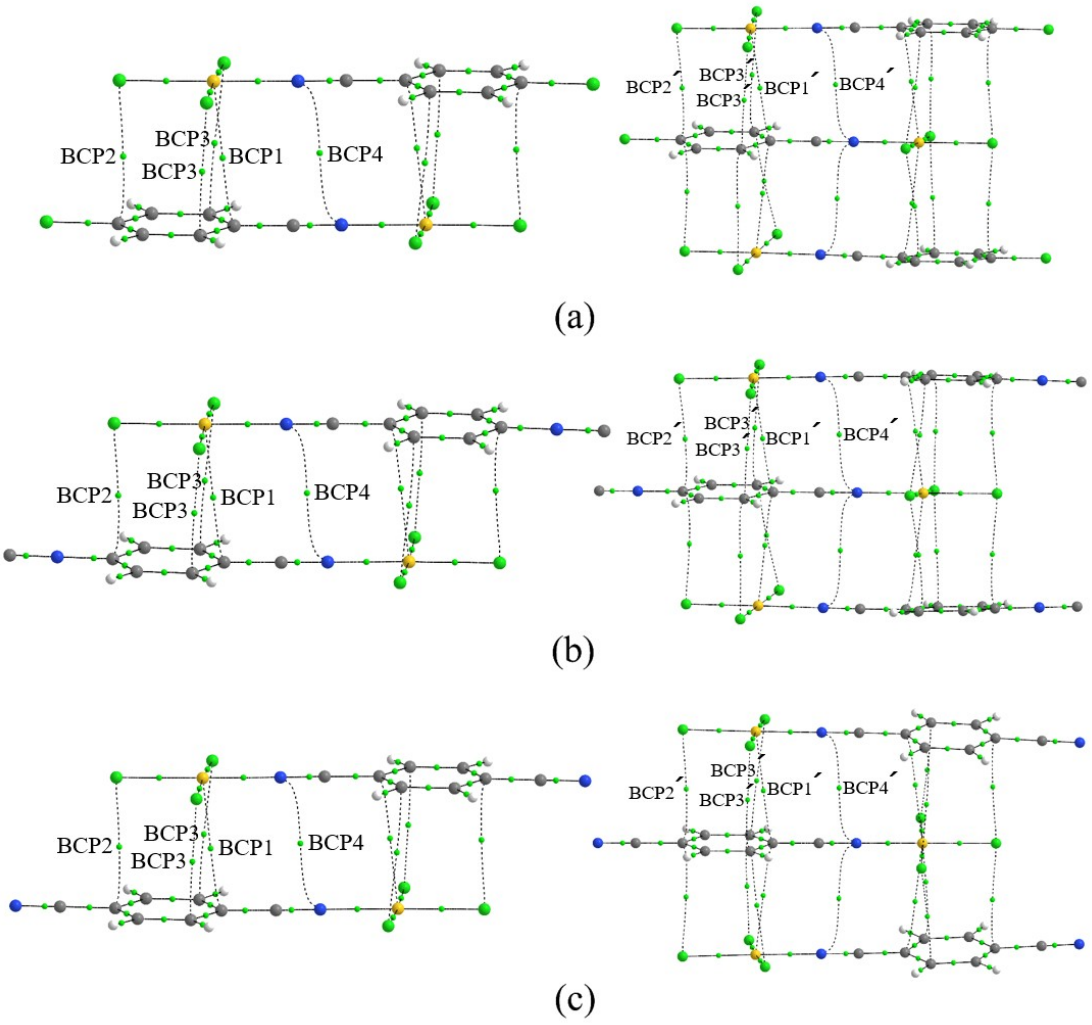

Fig. S4 AIM molecular graphs of the dimers and trimers (a)$(AuCl_3(NCC_6H_4Cl))_n$ (n = 2, 3); (b) $(AuCl_3(NCC_6H_4NC))_n$ (n = 2, 3); (c) $AuCl_3(NCC_6H_4CN))_n$ (n = 2, 3).