Electronic Supplementary Material for PCCP

Supplementary Material to: Density Functional Study of Aurophilic Interaction in $[X(AuPH_3)_2^+]_2$ (X=F, Cl, Br, I)

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Table S1 Bonding energy ΔE (in kJ/mol) decomposition of $[X(AuPH_3)_2^+]_2$ (X=F, Cl, Br, I) with different DF potentials; ΔE_1 for $[F(AuPH_3)_2^+]_2$; ΔE_2 for $[Cl(AuPH_3)_2^+]_2$; ΔE_3 for $[Br(AuPH_3)_2^+]_2$; ΔE_4 for $[I(AuPH_3)_2^+]_2$

ΔE_1							
	Xα	BLYP	VWN	BP	PW91	PBE	B3LYP
E_{pauli}	407.94	447.23	320.19	392.90	387.97	392.55	400.83
$E_{ele.}$	-108.45	-57.00	-54.82	-34.37	-41.60	-41.14	-25.18
$E_{ster.}$	299.50	390.22	265.38	358.53	346.37	351.41	375.65
$E_{orb.}$	-177.21	-153.98	-173.72	-163.14	-163.89	-163.75	-143.52
E_{tot}	122.29	236.24	91.66	195.39	182.47	187.67	232.13
ΔE_2							
	Xα	BLYP	VWN	BP	PW91	PBE	B3LYP
E_{pauli}	456.18	500.98	365.54	441.95	433.64	437.90	455.97
$E_{ele.}$	-144.32	-90.37	-91.60	-68.76	-74.54	-73.53	-61.34
$E_{ster.}$	311.86	410.61	273.94	373.19	359.10	364.37	394.63
$E_{orb.}$	-186.67	-162.76	-182.36	-171.53	-172.63	-172.49	-152.79
E_{tot}	125.20	247.85	91.57	201.66	186.47	191.88	241.83
ΔE_3							
	Xα	BLYP	VWN	BP	PW91	PBE	B3LYP

E_{pauli}	512.75	561.90	412.78	496.02	487.02	491.52	514.54
$E_{ele.}$	-188.38	-130.37	-129.46	-105.80	-112.73	-111.52	-99.85
$E_{ster.}$	324.38	431.53	283.33	390.22	374.29	380.00	414.69
$E_{orb.}$	-207.28	-181.78	-202.29	-190.73	-192.07	-192.01	-171.79
E_{tot}	117.10	249.75	81.03	199.49	182.22	187.99	242.90

ΔE_4

	Xα	BLYP	VWN	BP	PW91	PBE	B3LYP
E_{pauli}	541.12	593.98	435.04	523.66	511.40	517.27	547.57
$E_{ele.}$	-212.22	-151.02	-150.00	-126.04	-131.35	-131.44	-122.29
$E_{ster.}$	328.90	442.97	285.05	397.61	380.04	385.83	425.28
$E_{orb.}$	-216.97	-190.50	-211.45	-199.47	-201.13	-201.05	-181.32
E_{tot}	111.93	252.47	73.60	198.14	178.91	184.78	243.96

E_{Pauli}: Including exchange-correlation, i.e., the simulated dispersion attraction.

$E_{ele.}$: Hybridization, polarization, charge transfer, orbital interference.

$E_{ster.}$: Including Pauli repulsion and electrostatic interaction.

$E_{orb.}$: With respect to the monomeric structures as in the dimer.

$E_{tot.}$: Calculated binding energy.

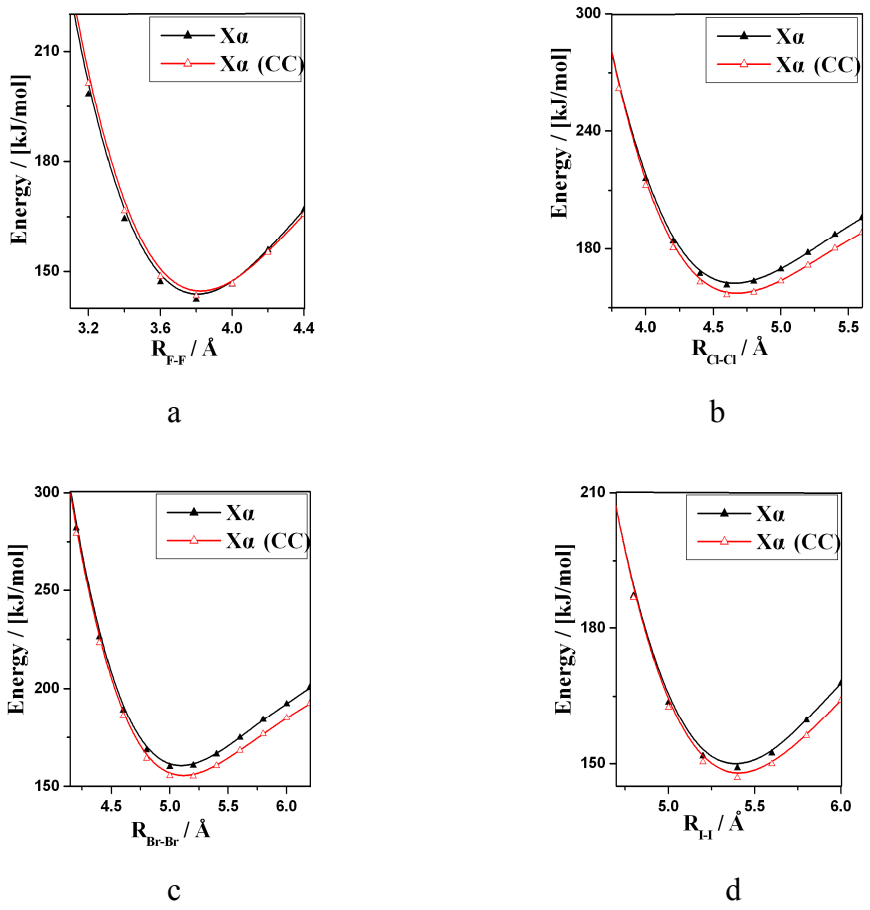

Fig. S1 The calculated binding energy (BE) (in kJ/mol) potential line between two relaxed $X(AuPH_3)_2^+$ units, with BSS-error: Xα, and corrected by the CC: Xα (CC), versus the X…X distance (in Å). a: $[F(AuPH_3)_2^+]_2$ b: $[Cl(AuPH_3)_2^+]_2$ c: $[Br(AuPH_3)_2^+]_2$ d: $[I(AuPH_3)_2^+]_2$.