Electronic Supplementary Material (ESI) for RSC Advances.

Table S1 Charge transfer (Q_{CT}, e) and second-order perturbation energy ($E^{(2)}$, kcal/mol) of tetrel bond in the triads as well as their difference (Δ) relative to the corresponding dyads

triads	Q_{CT}	ΔQ_{CT}	$E^{(2)}$	$\Delta E^{(2)}$
$C_2H_4\cdots AuCN\cdots CF_4$	-0.0016	-0.0031	0.11	0.02
$C_2H_4\cdots AuCN\cdots SiF_4$	-0.0148	-0.0138	11.76	8.53
$C_2H_4\cdots AuCN\cdots GeF_4$	-0.1239	-0.0238	90.25	18.08
$C_2H_4\cdots AuCN\cdots SnF_4$	-0.1203	-0.0113	91.02	8.75
$C_2H_4\cdots AgCN\cdots SiF_4$	-0.0992	-0.0376	64.94	24.78
$C_2H_4\cdots CuCN\cdots SiF_4$	-0.0789	-0.0676	---	---
$C_2(CN)_4\cdots AuCN\cdots SiF_4$	0.0010	0.0020	1.92	-0.31
$C_2(CN)_4\cdots AgCN\cdots SiF_4$	-0.0022	0.0594	4.20	-35.96
$C_2(CN)_4\cdots CuCN\cdots SiF_4$	0.0008	0.0121	---	---
$C_2H_2\cdots AuCN\cdots SiF_4$	-0.0132	-0.0122	10.86	7.63
$NCAu\cdots C_2H_4\cdots SiF_4$	0.0043	0.0049	---	---

Note: $E^{(2)}$ in the CuCN systems is not shown owing to the abnormal value in the NBO analysis. $E^{(2)}$ is not shown in $NCAu\cdots C_2H_4\cdots SiF_4$ due to the formation of covalent bond between C_2H_4 and AuCN.

Table S2 Electrostatic (E^{ele}), exchange (E^{ex}), repulsion (E^{rep}), polarization (E^{pol}), dispersion (E^{disp}) energies, and interaction energy (ΔE) of tetrel bond in the triads. All are in kcal/mol

triads	E^{ele}	E^{ex}	E^{rep}	E^{pol}	E^{disp}	ΔE
$C_2H_4\cdots AuCN\cdots CF_4$	-1.99	-2.95	5.11	-0.42	-1.09	-1.35
$C_2H_4\cdots AuCN\cdots SiF_4$	-19.02	-22.48	42.02	-6.43	-1.30	-7.21
$C_2H_4\cdots AuCN\cdots GeF_4$	-58.48	-64.02	131.72	-33.91	2.34	-22.35
$C_2H_4\cdots AuCN\cdots SnF_4$	-55.72	-56.95	115.51	-35.98	4.69	-28.46
$C_2H_4\cdots AgCN\cdots SiF_4$	-52.42	-60.87	121.38	-28.94	-0.71	-21.56
$C_2H_4\cdots CuCN\cdots SiF_4$	-44.82	-52.61	103.69	-23.04	-1.08	-17.87
$C_2(CN)_4\cdots AuCN\cdots SiF_4$	-8.70	-9.42	16.88	-2.01	-1.20	-4.45
$C_2(CN)_4\cdots AgCN\cdots SiF_4$	-13.11	-14.16	25.76	-3.44	-1.54	-6.49
$C_2(CN)_4\cdots CuCN\cdots SiF_4$	-9.60	-10.00	17.92	-2.23	-1.36	-5.27
$C_2H_2\cdots AuCN\cdots SiF_4$	-18.29	-21.55	40.20	-6.05	-1.31	-7.01
$NCAu\cdots C_2H_4\cdots SiF_4$	-4.31	-7.45	13.33	-0.57	-2.64	-1.64