First-Principles Study of Square Chalcogen Bond Interactions and its Adsorption Behavior on Silver Surface

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■ SUPPORTING INFORMATION

Fig S1. The symmetry-adapted perturbation theory (SAPT) calculations were carried out using PSI4 program, SAPT2+/aug-cc-PVDZ method is applied for energy decomposition calculations of dimer complexes, and SAPT2+/Def2-TZVPP method is applied for Te element. Energy units is in kcal/mol.

Table S1. Geometric parameters and the interaction energy E_{int} of dimers were calculated at MP2/aug-cc-pVTZ theory level. The %VDW denotes the ratio of d (Ch ⋯ N) to the sum of the VDW radii of two interacting atoms. d_1 and d_2 are the Ch ⋯ N chalcogen bond distance, respectively. The data in parentheses are the Ch⋯N distances of silver-surface supported dimer obtained using the PBE-D3 method.

Table S2. The optimized dimer structure using PBE-D3 method. %VDW is the ratio of d (Ch⋯N) to the sum of the VDW radii of the two interacting atoms. The data in parentheses are the Ch⋯N distances of silver-surface supported dimer obtained using the PBE-D3 method.

Table S3. The single point energy E_{int} (kcal/mol) of the dimer complex calculated at DLPNO-CCSD(T) theory level. %VDW denotes the ratio of d (Ch⋯N) to the sum of the VDW radii of the two interacting atoms. d_1 and d_2 are the Ch⋯N chalcogen bond distance, respectively. The data in parentheses are the Ch⋯N distances of silver-surface supported dimer obtained using the PBE-D3 method.

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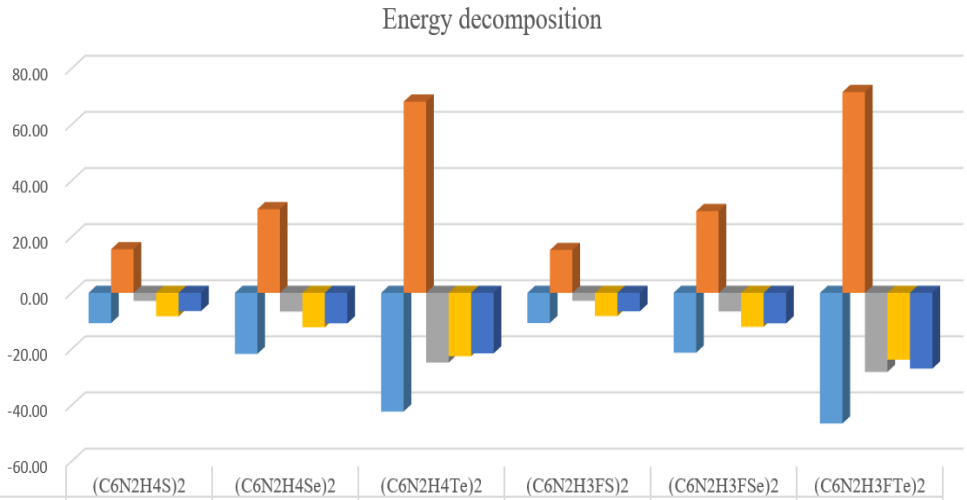
Fig S1. The symmetry-adapted perturbation theory (SAPT) calculations were carried out using PSI4 program, SAPT2+/aug-cc-PVDZ method is applied for energy decomposition calculations of dimer complexes, and SAPT2+/Def2-TZVPP method is applied for Te element. Energy unit is in kcal/mol.



	(C6N2H4S)2	(C6N2H4Se)2	(C6N2H4Te)2	(C6N2H3FS)2	(C6N2H3FSe)2	(C6N2H3FTe)2
Electrostatics (kcal/mol)	-10.79	-21.76	-42.31	-10.73	-21.31	-46.56
Exchange(kcal/mol)	15.54	29.81	68.15	15.27	29.15	71.58
Induction(kcal/mol)	-2.89	-6.66	-24.84	-2.83	-6.62	-28.18
Dispersion(kcal/mol)	-8.35	-12.23	-22.57	-8.26	-12.08	-23.82
Total interaction energy(kcal/mol)	-6.49	-10.84	-21.57	-6.55	-10.86	-26.98

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Complexes	d_1 (Å)	d_2 (Å)	%vdW	E_{int} (kcal/mol)
$(C_6N_2H_4S)_2$	2.969 (2.858)	2.969 (3.213)	0.919	-6.693
$(C_6N_2H_4Se)_2$	2.841 (2.720)	2.841 (2.753)	0.851	-7.548
$(C_6N_2H_3FS)_2$	2.970 (2.893)	2.971 (3.164)	0.920	-5.188
$(C_6N_2H_3FSe)_2$	2.843 (2.649)	2.846 (2.841)	0.852	-7.592

Table S2. The optimized dimer structure using PBE-D3 method. %VDW is the ratio of d (Ch···N) to the sum of the VDW radii of the two interacting atoms. The data in parentheses are the Ch···N distances of silver-surface supported dimer obtained using the PBE-D3 method.

Complexes	d_1 (Å)	d_2 (Å)	%vdW	E_{int} (kcal/mol)
$(C_6N_2H_4S)_2$	3.206 (2.858)	3.200 (3.213)	0.992	-3.851
$(C_6N_2H_4Se)_2$	2.862 (2.720)	2.859 (2.753)	0.856	-7.818
$(C_6N_2H_4Te)_2$	2.563 (2.428)	2.562 (2.454)	0.704	-18.379
$(C_6N_2H_3FS)_2$	3.117 (2.893)	3.112 (3.164)	0.964	-3.989
$(C_6N_2H_3FSe)_2$	2.841 (2.649)	2.838 (2.841)	0.850	-8.071
$(C_6N_2H_3FTe)_2$	2.532 (2.370)	2.531 (2.453)	0.695	-19.071

Table S3. The single point energy E_{int} (kcal/mol) of the dimer complex calculated at DLPNO-CCSD(T) theory level. %VDW denotes the ratio of d (Ch···N) to the sum of the VDW radii of the two interacting atoms. d_1 and d_2 are the Ch···N chalcogen bond distance, respectively. The data in parentheses are the Ch···N distances of silver-surface supported dimer obtained using the PBE-D3 method.

Complexes	d_1 (Å)	d_2 (Å)	%vdW	E_{int} (kcal/mol)
$(C_6N_2H_4S)_2$	3.077 (2.858)	3.077 (3.213)	0.953	-4.499
$(C_6N_2H_4Se)_2$	2.845 (2.720)	2.845 (2.753)	0.852	-7.141
$(C_6N_2H_4Te)_2$	2.564 (2.428)	2.564 (2.454)	0.704	-14.049
$(C_6N_2H_3FS)_2$	3.074 (2.893)	3.074 (3.164)	0.952	-4.621
$(C_6N_2H_3FSe)_2$	2.830 (2.649)	2.831 (2.841)	0.847	-7.379
$(C_6N_2H_3FTe)_2$	2.557 (2.370)	2.557 (2.453)	0.702	-17.039