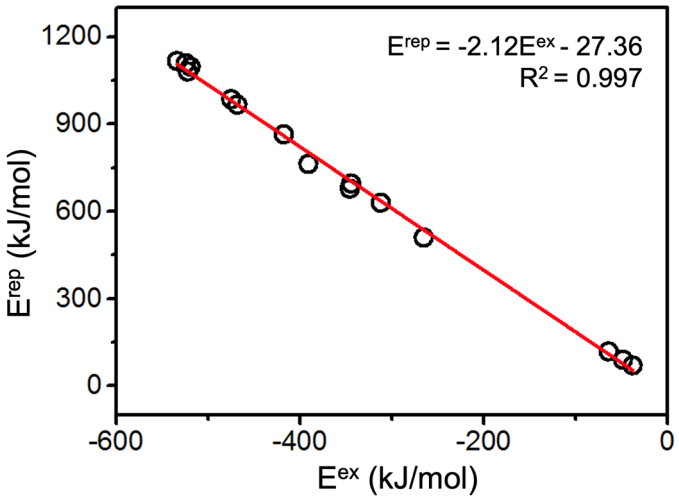

Figure S1. The relationship between repulsion energy E^{rep} and exchange energy E^{ex} in the complexes between Y_2CTe (Y = H, F, and CH_3) and XF (X = H, F, Cl, Br, and I).

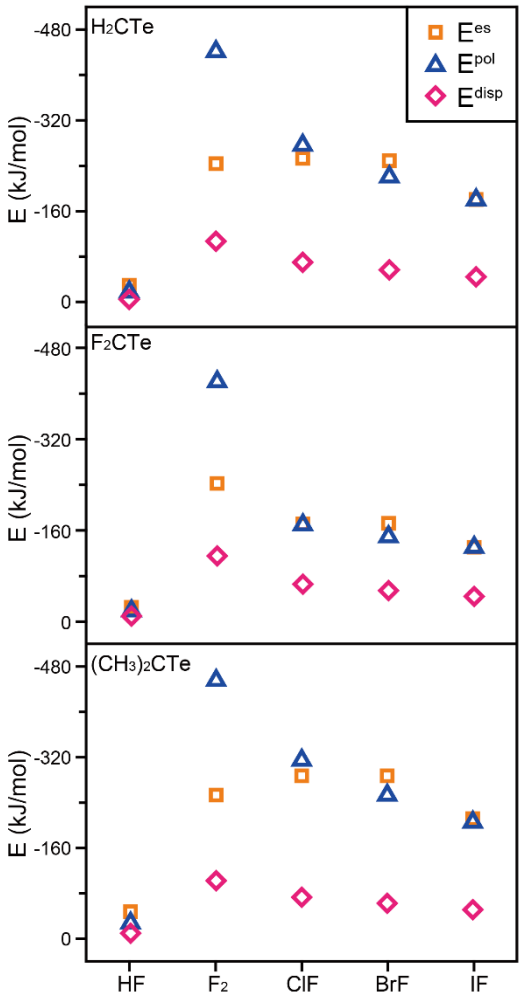

Figure S2. Electrostatic (E^{es}), polarization (E^{pol}), and dispersion (E^{disp}) energies in complexes between Y_2CTe (Y = H, F, and CH_3) and XF (X = H, F, Cl, Br, and I).

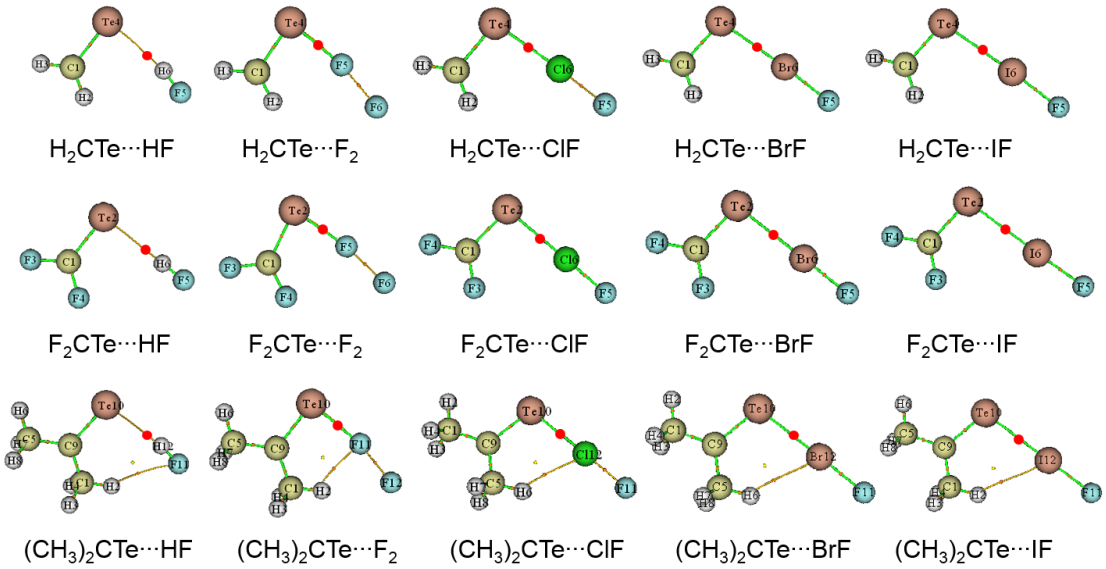

Figure S3. Molecular graphs of the complexes between Y_2CTe (Y = H, F, CH_3) and XF (X = H, F, Cl, Br, I). Small red balls indicate the Te···X bond critical point.

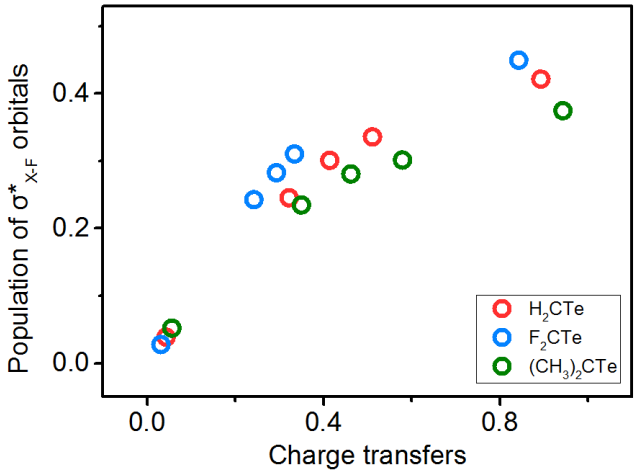

Figure S4. The relationship between the population of the $\sigma^*_{x\text{-}F}$ orbitals and the charge transfer in the complexes formed by Y_2CTe (Y = H, F, and CH_3) and XF (X = H, F, Cl, Br, and I).

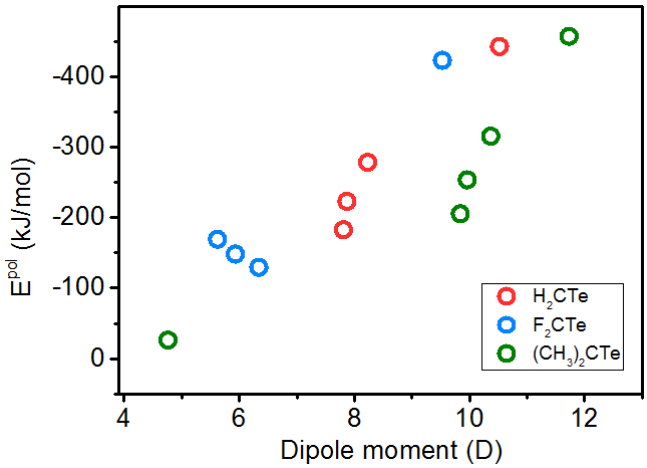

Figure S5. The relationship between the polarization energy E^{pol} and the dipole moment of the complexes formed by Y_2CTe (Y = H, F, and CH_3) and XF (X = F, Cl, Br, and I).

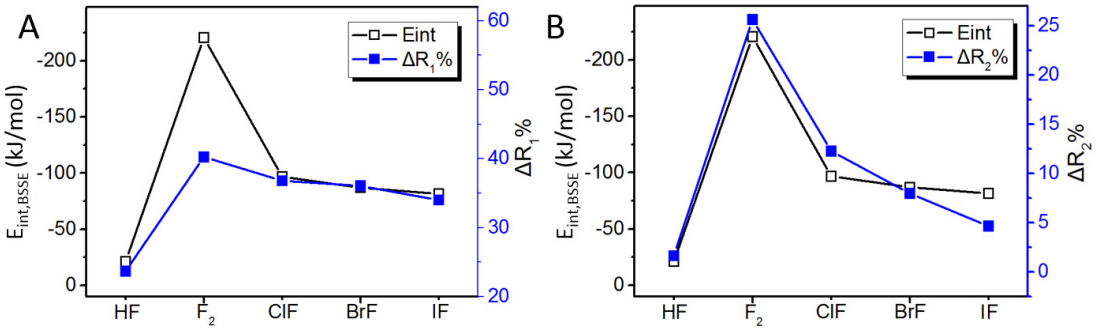

Figure S6. Trend comparison of $E_{int,BSSE}$ with ΔR_1% (A) and ΔR_2% (B) in $H_2CTe\cdots XF$ systems.

The coordinates of optimized monomer Y_2CTe (Y = H, F, CH_3), XF (X = H, F, Cl, Br, I), and their complexes.

H_2CTe

C	0.00000000	-1.66932500	0.00000000
H	0.92452000	-2.23381100	0.00000000
H	-0.92451100	-2.23383600	0.00000000
Te	0.00000000	0.27853100	0.00000000

F_2CTe

C	-0.00017100	-1.14712200	0.00000000
Te	0.00000000	0.79898600	0.00000000
F	-1.06263500	-1.92596600	0.00000000
F	1.06274800	-1.92564800	0.00000000

$(CH_3)_2CTe$

C	1.93856200	-1.26029100	-0.00000500
H	1.31811300	-2.15179700	0.00023300
H	2.59352800	-1.27798900	-0.87673500
H	2.59369100	-1.27772700	0.87664400
C	1.93856200	1.26029100	-0.00000500
H	1.31811200	2.15179700	0.00018800
H	2.59365900	1.27774900	0.87666700
H	2.59356100	1.27796800	-0.87671100
C	1.13007900	0.00000000	-0.00004300
Te	-0.82795900	0.00000000	0.00000100

HF

F	0.00000000	0.00000000	0.09218500
H	0.00000000	0.00000000	-0.82966400

F_2

F	0.00000000	0.00000000	0.70058100
F	0.00000000	0.00000000	-0.70058100

ClF

F	0.00000000	0.00000000	-1.07141000
Cl	0.00000000	0.00000000	0.56721700

BrF

F	0.00000000	0.00000000	-1.39848000
Br	0.00000000	0.00000000	0.35960900

IF

F	0.00000000	0.00000000	-1.64106200
I	0.00000000	0.00000000	0.27867100

$H_2CTe\cdots HF$

C	0.40812600	1.67368900	0.00000100
H	-0.54068900	2.19616900	0.00002900
H	1.31096600	2.27166100	-0.00002800
Te	0.48693200	-0.27130600	0.00000000
F	-2.94540300	-0.01992700	-0.00000400
H	-2.03088400	-0.22270500	0.00002600

$H_2CTe\cdots F_2$

C	0.51970200	1.67251800	0.00002200
H	-0.48672200	2.07748600	0.00022600
H	1.37653600	2.33277200	-0.00015500
Te	0.71822400	-0.24278900	-0.00001800
F	-1.43262200	-0.26363900	0.00020500
F	-3.16245400	0.06137700	-0.00012500

$H_2CTe\cdots ClF$

C	-1.25498700	1.62469400	-0.00006500
H	-0.41452400	2.31006100	-0.00044800
H	-2.26293200	2.01928900	0.00060000
Te	-0.91890200	-0.28308800	0.00005700
F	3.42150000	0.19550700	0.00047500
Cl	1.59981200	-0.06567700	-0.00041200

$H_2CTe\cdots BrF$

C	1.65383900	1.61692300	0.00009200
H	0.83845500	2.33141600	-0.00054900
H	2.67380200	1.97959400	0.00011700
Te	1.26240200	-0.28281600	0.00000400
F	-3.29294600	0.22141800	0.00008800
Br	-1.41267700	-0.03711000	-0.00003200

$H_2CTe\cdots IF$

C	2.01881700	1.61089600	-0.00004800
H	1.22353500	2.34720300	0.00017000
H	3.04781300	1.94746100	0.00009500
Te	1.58697200	-0.28253200	-0.00001900
F	-3.29898500	0.22575100	-0.00016700
I	-1.30596000	-0.02453100	0.00004800

$F_2CTe\cdots HF$

C	1.08366000	0.73214800	-0.00000800
Te	-0.12459800	-0.79958200	-0.00006800
F	2.39464000	0.67109600	0.00066800
F	0.73141600	1.99450700	-0.00066100
F	-2.88903700	1.37711700	0.00043200
H	-2.15602300	0.80089100	-0.00037400

$F_2CTe\cdots F_2$

C	0.68580800	1.14353100	0.00010600
Te	0.47860400	-0.80989200	0.00001200
F	1.84938300	1.73902900	-0.00019500
F	-0.26276700	2.01553500	0.00017100
F	-1.59342000	-0.27577200	-0.00002600
F	-3.21566600	0.43822900	-0.00008800

$F_2CTe\cdots ClF$

C	1.33414700	0.95989900	-0.00001000
Te	0.53636300	-0.82911500	-0.00001000
F	0.68265900	2.08546600	-0.00023500
F	2.62071700	1.20135800	0.00025300
F	-3.61192200	0.70552900	0.00022400
Cl	-1.94816700	0.08372900	-0.00009400

$F_2CTe\cdots BrF$

C	-1.68704400	0.96627900	0.00062800
Te	-0.89839900	-0.82677600	-0.00008400
F	-1.03167800	2.09068700	-0.00066500
F	-2.97261900	1.21346600	0.00040700
F	3.51394400	0.62883100	0.00013200
Br	1.75006300	0.05136700	0.00004900

$F_2CTe\cdots IF$

C	-2.02087300	0.97456600	0.00010700
Te	-1.23738400	-0.82094400	0.00007200
F	-1.36556400	2.09979500	-0.00269300
F	-3.30660300	1.22305500	0.00298500
F	3.54311400	0.57406800	0.00425600
I	1.63454100	0.03338500	-0.00085500

$(CH_3)_2CTe\cdots HF$

C	-0.68363000	2.12169900	-0.00005900
H	0.39320300	2.26186800	-0.00050600
H	-1.11097000	2.62003100	-0.87580900
H	-1.11015900	2.61976100	0.87623500

C	-2.57337200	0.45359000	0.00006300
H	-2.83391000	-0.60092200	0.00033700
H	-3.01824200	0.93473100	0.87639400
H	-3.01825300	0.93426600	-0.87651200
C	-1.09553900	0.68486600	-0.00003400
Te	0.18246200	-0.80007500	-0.00000600
F	2.79696000	1.39584500	0.00005700
H	2.15293100	0.71064800	-0.00015000

$(CH_3)_2CTe\cdots F_2$

C	0.00709700	2.15778100	0.00031500
H	1.05438900	1.86921100	-0.00309000
H	-0.21188300	2.78120700	-0.87251500
H	-0.20652400	2.77505300	0.87897900
C	-2.38518400	1.32179000	-0.00038300
H	-3.02254400	0.44135600	-0.00132800
H	-2.61746300	1.93179600	0.87718700
H	-2.61697700	1.93361200	-0.87670200
C	-0.92595300	1.00005900	-0.00030000
Te	-0.32703800	-0.85460500	0.00002400
F	1.72569500	-0.13125500	0.00030200
F	3.21332900	0.77897000	-0.00047800

$(CH_3)_2CTe\cdots ClF$

C	2.92247500	0.87353200	0.00008200
H	3.35275400	-0.12518200	-0.00016400
H	3.28370800	1.41839500	-0.87681900
H	3.28353400	1.41784300	0.87740700
C	0.76078800	2.19989800	-0.00007300
H	-0.32356400	2.13202900	-0.00007100
H	1.09027500	2.76548500	0.87692300
H	1.09032400	2.76548200	-0.87703600
C	1.42889600	0.87080800	-0.00003500
Te	0.43868800	-0.81687500	-0.00001200
F	-3.63261700	0.79339600	0.00003800
Cl	-1.91577700	0.07632000	0.00001200

$(CH_3)_2CTe\cdots BrF$

C	3.27124700	0.89441800	-0.00000500
H	3.70841000	-0.10122500	-0.00038200
H	3.62881000	1.44210900	-0.87672900
H	3.62870800	1.44131200	0.87728200
C	1.09925100	2.20323500	-0.00000800
H	0.01569400	2.12093400	-0.00026900

H	1.42104200	2.77266600	0.87736100
H	1.42153400	2.77285300	-0.87707900
C	1.77777000	0.87948800	-0.00001600
Te	0.79941100	-0.81666500	-0.00000800
F	-3.53051000	0.70451400	-0.00005700
Br	-1.72881700	0.05184100	0.00002600

$(CH_3)_2CTe\cdots IF$

C	1.44947400	2.21367000	0.00006600
H	0.36497200	2.13948200	0.00072500
H	1.77466200	2.78222700	0.87686300
H	1.77344700	2.78163300	-0.87757300
C	3.61290500	0.89578700	-0.00005500
H	4.04605500	-0.10147400	0.00054100
H	3.97255200	1.44120800	-0.87746900
H	3.97278300	1.44248900	0.87644400
C	2.11895600	0.88530300	0.00005000
Te	1.13887600	-0.81134900	0.00001800
F	-3.55773600	0.63235600	0.00004500
I	-1.62631000	0.03858100	-0.00002300