Supplementary Material (ESI) for PCCP

Supporting Information

The Isomeric Effect on the Adjacent Si Dimer Didechlorination of *trans* and *iso*-Dichloroethylene on Si(100)-2×1

Qiuju Zhang, Bo Li, Qinghong Yuan, Baihai Li, Zhifeng Liu, and Liang Chen

[1] Atomic coordinates and electronic energies of adsorption structures for *trans*-DCE single and double dechlorination on Si(100)

[2] Atomic coordinates and electronic energies of adsorption structures for *iso*-DCE single and double dechlorination on Si(100)

[3] Imaginary vibrational frequencies of the transition states along single and double dechlorination processes of *trans* and *iso*-DCE dissociation on Si(100)

[1] The Cartesian coordinates and electronic energies (GGA-PW91) of adsorption structures for single and double dechlorination of *trans*-DCE on Si(100) using *p*(2×2) unit cell and (4×2) supercell.

mono-σ^A (E= -161.839052 eV)

C	0.266050000	0.944100000	8.069500000
C	7.642670000	1.981510000	8.844420000
H	0.390100000	7.649400000	8.521070000
H	7.522840000	3.005080000	8.488980000
H	0.000000000	0.000000000	0.000000000
H	0.000000000	2.280000000	0.000000000
H	0.000000000	3.847000000	0.000000000
H	0.000000000	6.127000000	0.000000000
H	3.847000000	0.000000000	0.000000000
H	3.847000000	2.280000000	0.000000000
H	3.847000000	3.847000000	0.000000000
H	3.847000000	6.127000000	0.000000000
Si	0.000000000	1.140000000	0.930000000
Si	0.000000000	4.987000000	0.930000000
Si	3.847000000	1.140000000	0.930000000
Si	3.847000000	4.987000000	0.930000000
Si	1.929540000	1.102730000	2.191590000
Si	1.919690000	4.943990000	2.221690000
Si	5.778170000	1.104030000	2.330510000
Si	5.773010000	4.946900000	2.319250000
Si	1.891420000	3.001190000	3.535180000
Si	1.896330000	6.881980000	3.515080000
Si	5.809640000	3.026680000	3.745870000
Si	5.812520000	6.857300000	3.732630000
Si	0.111740000	3.058290000	5.071020000
Si	0.117810000	6.818870000	5.039990000
Si	3.778940000	2.962010000	4.989690000
Si	3.778370000	6.878640000	4.965720000
Si	0.661510000	1.077870000	6.254220000
Si	0.563360000	4.950410000	6.464700000
Si	3.083160000	1.060290000	6.196190000
Si	2.769130000	4.921770000	5.750540000
Cl	3.883710000	1.027390000	8.123530000
Cl	7.402830000	1.856010000	10.558370000

mono-σ^B (E= -161.810237 eV)

C	3.430020000	1.953820000	8.972660000
C	3.557440000	0.952950000	8.099160000

H	3.083200000	2.955260000	8.718940000
H	3.903300000	7.674970000	8.459530000
H	0.000000000	0.000000000	0.000000000
H	0.000000000	2.280000000	0.000000000
H	0.000000000	3.847000000	0.000000000
H	0.000000000	6.127000000	0.000000000
H	3.847000000	0.000000000	0.000000000
H	3.847000000	2.280000000	0.000000000
H	3.847000000	3.847000000	0.000000000
H	3.847000000	6.127000000	0.000000000
Si	0.000000000	1.140000000	0.930000000
Si	0.000000000	4.987000000	0.930000000
Si	3.847000000	1.140000000	0.930000000
Si	3.847000000	4.987000000	0.930000000
Si	1.928070000	1.102860000	2.193080000
Si	1.921120000	4.948020000	2.225330000
Si	5.767880000	1.109170000	2.335650000
Si	5.752900000	4.954640000	2.325660000
Si	1.876520000	3.002330000	3.535210000
Si	1.869450000	6.885520000	3.524840000
Si	5.750680000	3.032000000	3.751790000
Si	5.750360000	6.864900000	3.746800000
Si	0.067840000	3.074360000	5.029950000
Si	0.065320000	6.783550000	5.026920000
Si	3.727540000	2.951930000	5.040380000
Si	3.719030000	6.912120000	5.015280000
Si	0.591550000	1.076870000	6.177010000
Si	0.510030000	4.928900000	6.476830000
Si	3.023820000	1.071960000	6.311300000
Si	2.714930000	4.930910000	5.754170000
Cl	3.787400000	1.809390000	10.662490000
Cl	7.468330000	1.073510000	8.102860000

di-σ (E= -289.909267 eV)

C	1.141330000	5.154510000	8.043010000
C	2.674770000	4.987090000	8.031840000
H	0.875130000	6.176570000	8.342250000
H	2.965070000	4.020610000	8.461250000
H	0.000000000	0.000000000	0.000000000
H	0.000000000	2.280000000	0.000000000
H	0.000000000	3.847000000	0.000000000
H	0.000000000	6.127000000	0.000000000
H	3.847000000	0.000000000	0.000000000
H	3.847000000	2.280000000	0.000000000

H	3.847000000	3.847000000	0.000000000
H	3.847000000	6.127000000	0.000000000
H	0.000000000	7.701000000	0.000000000
H	0.000000000	9.981000000	0.000000000
H	3.847000000	7.701000000	0.000000000
H	3.847000000	9.981000000	0.000000000
H	0.000000000	11.548000000	0.000000000
H	0.000000000	13.828000000	0.000000000
H	3.847000000	11.548000000	0.000000000
H	3.847000000	13.828000000	0.000000000
Si	0.000000000	1.140000000	0.930000000
Si	0.000000000	4.987000000	0.930000000
Si	3.847000000	1.140000000	0.930000000
Si	3.847000000	4.987000000	0.930000000
Si	0.000000000	8.820000000	0.930000000
Si	0.000000000	12.667000000	0.930000000
Si	3.847000000	8.820000000	0.930000000
Si	3.847000000	12.667000000	0.930000000
Si	1.918280000	1.141030000	2.215930000
Si	1.927670000	4.976500000	2.215530000
Si	5.764090000	1.119720000	2.328390000
Si	5.776610000	4.975690000	2.343320000
Si	1.890300000	3.057000000	3.556390000
Si	1.888590000	6.897020000	3.541110000
Si	5.800430000	3.029400000	3.749880000
Si	5.797880000	6.922960000	3.740710000
Si	0.093180000	2.940000000	5.080230000
Si	0.092180000	6.988630000	5.055940000
Si	3.783460000	3.062410000	5.014260000
Si	3.778630000	6.914580000	4.995270000
Si	0.576970000	1.102850000	6.545310000
Si	0.674120000	4.968400000	6.138930000
Si	2.791900000	1.084640000	5.780630000
Si	3.031760000	4.999740000	6.113470000
Si	1.916980000	8.812760000	2.212480000
Si	5.763000000	8.832990000	2.327120000
Si	1.917250000	10.736640000	3.546840000
Si	5.761830000	10.741300000	3.776400000
Si	0.083800000	10.627010000	5.068910000
Si	3.745320000	10.868650000	5.079470000
Si	0.559530000	8.810150000	6.552730000
Si	2.788820000	8.866510000	5.809970000
Si	1.933490000	12.659820000	2.209850000
Si	5.776630000	12.661850000	2.344650000

Si	1.923700000	14.590830000	3.526290000
Si	5.768650000	14.589470000	3.763010000
Si	0.096670000	14.687310000	5.045990000
Si	3.749170000	14.470000000	5.056110000
Si	1.001780000	12.657360000	5.783290000
Si	3.233430000	12.677980000	6.559390000
Cl	0.308290000	4.069950000	9.222830000
Cl	3.544130000	6.243950000	9.000440000

end-bridge (E = -289.793100 eV)

C	8.009450000	2.341460000	7.889120000
C	8.273790000	3.877880000	7.916220000
H	8.449820000	1.904060000	8.794340000
H	7.527460000	4.341480000	8.574210000
H	7.694000000	0.000000000	0.000000000
H	7.694000000	2.280000000	0.000000000
H	7.694000000	3.847000000	0.000000000
H	7.694000000	6.127000000	0.000000000
H	11.541000000	0.000000000	0.000000000
H	11.541000000	2.280000000	0.000000000
H	11.541000000	3.847000000	0.000000000
H	11.541000000	6.127000000	0.000000000
H	3.854000000	0.000000000	0.000000000
H	3.854000000	2.280000000	0.000000000
H	3.854000000	3.847000000	0.000000000
H	3.854000000	6.127000000	0.000000000
H	0.014000000	0.000000000	0.000000000
H	0.014000000	2.280000000	0.000000000
H	0.014000000	3.847000000	0.000000000
H	0.014000000	6.127000000	0.000000000
Si	11.541000000	1.140000000	0.930000000
Si	11.541000000	4.987000000	0.930000000
Si	3.854000000	1.140000000	0.930000000
Si	3.854000000	4.987000000	0.930000000
Si	7.701000000	1.140000000	0.930000000
Si	7.701000000	4.987000000	0.930000000
Si	0.014000000	1.140000000	0.930000000
Si	0.014000000	4.987000000	0.930000000
Si	9.627910000	1.082090000	2.235760000
Si	9.615910000	5.022880000	2.214720000
Si	13.487150000	1.126810000	2.323130000
Si	13.466340000	4.981270000	2.318190000
Si	9.676250000	3.066810000	3.447470000
Si	9.563320000	6.874890000	3.680840000

Si	13.500060000	3.056220000	3.721230000
Si	13.477570000	6.896030000	3.747950000
Si	7.790940000	3.021760000	4.783620000
Si	7.758750000	6.977560000	5.289850000
Si	11.497490000	2.921520000	4.979530000
Si	11.492200000	7.044100000	5.079720000
Si	8.594410000	1.378310000	6.270710000
Si	8.382170000	4.799760000	6.169180000
Si	11.012990000	1.186080000	6.539190000
Si	10.736220000	4.962680000	5.779380000
Si	5.773030000	1.109120000	2.323810000
Si	5.769290000	5.009870000	2.350130000
Si	5.720190000	3.042200000	3.687600000
Si	5.795910000	6.924870000	3.831260000
Si	3.762500000	2.930600000	5.065760000
Si	3.751690000	7.020470000	5.068010000
Si	3.208800000	1.129100000	6.553900000
Si	2.859260000	4.973920000	5.774850000
Si	1.943580000	1.130850000	2.210960000
Si	1.926310000	4.976030000	2.211430000
Si	1.937880000	3.051810000	3.541700000
Si	1.932640000	6.899870000	3.539770000
Si	0.099180000	3.162340000	5.042840000
Si	0.094600000	6.774020000	5.049300000
Si	0.984560000	1.120120000	5.763580000
Si	0.623030000	4.965270000	6.540790000
Cl	6.209580000	2.086770000	8.052070000
Cl	9.876070000	4.186250000	8.752650000

intra dimer tetra-σ (E = -292.940196 eV)

C	1.227000000	5.017200000	7.953000000
C	2.580460000	4.972740000	7.954610000
H	0.618350000	5.058990000	8.861100000
H	3.197590000	4.961030000	8.857210000
H	0.000000000	0.000000000	0.000000000
H	0.000000000	2.280000000	0.000000000
H	0.000000000	3.847000000	0.000000000
H	0.000000000	6.127000000	0.000000000
H	3.847000000	0.000000000	0.000000000
H	3.847000000	2.280000000	0.000000000
H	3.847000000	3.847000000	0.000000000
H	3.847000000	6.127000000	0.000000000
H	0.000000000	7.701000000	0.000000000
H	0.000000000	9.981000000	0.000000000

H	3.847000000	7.701000000	0.000000000
H	3.847000000	9.981000000	0.000000000
H	0.000000000	11.548000000	0.000000000
H	0.000000000	13.828000000	0.000000000
H	3.847000000	11.548000000	0.000000000
H	3.847000000	13.828000000	0.000000000
Si	0.000000000	1.140000000	0.930000000
Si	0.000000000	4.987000000	0.930000000
Si	3.847000000	1.140000000	0.930000000
Si	3.847000000	4.987000000	0.930000000
Si	0.000000000	8.820000000	0.930000000
Si	0.000000000	12.667000000	0.930000000
Si	3.847000000	8.820000000	0.930000000
Si	3.847000000	12.667000000	0.930000000
Si	1.923340000	1.162040000	2.205840000
Si	1.924410000	5.020230000	2.229740000
Si	5.766600000	1.121200000	2.315390000
Si	5.775590000	5.016220000	2.321080000
Si	1.904820000	3.067350000	3.540600000
Si	1.904850000	6.940020000	3.562980000
Si	5.786630000	3.058620000	3.679860000
Si	5.785720000	6.936680000	3.750100000
Si	0.050450000	3.078310000	5.009570000
Si	0.082710000	7.042550000	5.048390000
Si	3.814050000	3.090920000	4.977070000
Si	3.767570000	6.951950000	5.004930000
Si	0.678720000	1.133630000	6.178870000
Si	0.702560000	5.044060000	6.123250000
Si	3.047190000	1.080450000	5.821740000
Si	3.070250000	5.006490000	6.123340000
Si	1.916300000	8.834140000	2.209400000
Si	5.764960000	8.836040000	2.325420000
Si	1.930270000	10.749370000	3.568470000
Si	5.760670000	10.734490000	3.790980000
Si	0.079590000	10.578190000	5.086800000
Si	3.730540000	10.763640000	5.064120000
Si	0.615280000	8.802680000	6.574190000
Si	3.046190000	8.825990000	6.253340000
Si	1.932410000	12.675270000	2.239440000
Si	5.775600000	12.634520000	2.333070000
Si	1.933740000	14.648950000	3.553320000
Si	5.761190000	14.571040000	3.715850000
Si	0.055480000	14.579520000	5.010500000
Si	3.797700000	14.421670000	5.065550000

Si	1.023190000	12.586650000	5.772410000
Si	3.252530000	12.612020000	6.505640000
Cl	0.122000000	1.170760000	8.192040000
Cl	4.032800000	8.781930000	8.113470000

inter dimer tetra-σ_I （E = -292.936973 eV）

C	7.934040000	2.357530000	7.820440000
C	7.938870000	3.716760000	7.838260000
H	7.755870000	1.836420000	8.767830000
H	7.768150000	4.218370000	8.796340000
H	7.694000000	0.000000000	0.000000000
H	7.694000000	2.280000000	0.000000000
H	7.694000000	3.847000000	0.000000000
H	7.694000000	6.127000000	0.000000000
H	11.541000000	0.000000000	0.000000000
H	11.541000000	2.280000000	0.000000000
H	11.541000000	3.847000000	0.000000000
H	11.541000000	6.127000000	0.000000000
H	3.854000000	0.000000000	0.000000000
H	3.854000000	2.280000000	0.000000000
H	3.854000000	3.847000000	0.000000000
H	3.854000000	6.127000000	0.000000000
H	0.014000000	0.000000000	0.000000000
H	0.014000000	2.280000000	0.000000000
H	0.014000000	3.847000000	0.000000000
H	0.014000000	6.127000000	0.000000000
Si	11.541000000	1.140000000	0.930000000
Si	11.541000000	4.987000000	0.930000000
Si	3.854000000	1.140000000	0.930000000
Si	3.854000000	4.987000000	0.930000000
Si	7.701000000	1.140000000	0.930000000
Si	7.701000000	4.987000000	0.930000000
Si	0.014000000	1.140000000	0.930000000
Si	0.014000000	4.987000000	0.930000000
Si	9.621610000	1.074770000	2.227570000
Si	9.617570000	5.028540000	2.217660000
Si	13.474040000	1.126760000	2.323460000
Si	13.459840000	4.978390000	2.311460000
Si	9.697380000	3.054420000	3.414690000
Si	9.536510000	6.895360000	3.666410000
Si	13.450780000	3.057270000	3.717810000
Si	13.417770000	6.890280000	3.735830000
Si	7.844980000	3.057070000	4.760230000

Si	7.752160000	6.895200000	5.306280000
Si	11.449260000	3.010460000	4.986180000
Si	11.423440000	6.918280000	5.057280000
Si	8.422260000	1.353390000	6.260960000
Si	8.397780000	4.740910000	6.281330000
Si	10.832790000	1.147360000	6.284250000
Si	10.822960000	4.935940000	6.202120000
Si	5.778320000	1.103340000	2.325530000
Si	5.774080000	5.005930000	2.317350000
Si	5.774950000	3.058960000	3.661100000
Si	5.832760000	6.892930000	3.804590000
Si	3.809670000	3.018560000	5.008710000
Si	3.781480000	6.919130000	4.998540000
Si	3.076080000	1.120690000	6.192200000
Si	2.776840000	4.965130000	5.718110000
Si	1.934880000	1.126180000	2.209780000
Si	1.933380000	4.968790000	2.252240000
Si	1.918810000	3.014250000	3.566260000
Si	1.899210000	6.924860000	3.556690000
Si	0.048770000	3.147710000	5.016370000
Si	0.035080000	6.782590000	5.017420000
Si	0.732020000	1.117800000	5.848050000
Si	0.577320000	4.964580000	6.480680000
Cl	3.643590000	1.128120000	8.202430000
Cl	11.594170000	4.899860000	8.153290000

[2] Cartesian coordinates and electronic energies of adsorption structures for single and double dechlorination of *iso*-DCE on Si(100)

mono-σ^{B} (E = -161.730232 eV)

C	3.544040000	1.018370000	8.071410000
C	3.205930000	1.991070000	8.920170000
H	2.666870000	2.865480000	8.552800000
H	3.419190000	1.946740000	9.986740000
H	0.000000000	0.000000000	0.000000000
H	0.000000000	2.280000000	0.000000000
H	0.000000000	3.847000000	0.000000000
H	0.000000000	6.127000000	0.000000000
H	3.847000000	0.000000000	0.000000000
H	3.847000000	2.280000000	0.000000000
H	3.847000000	3.847000000	0.000000000
H	3.847000000	6.127000000	0.000000000
Si	0.000000000	1.140000000	0.930000000
Si	0.000000000	4.987000000	0.930000000

Si	3.847000000	1.140000000	0.930000000
Si	3.847000000	4.987000000	0.930000000
Si	1.928460000	1.102330000	2.192000000
Si	1.921900000	4.947770000	2.218310000
Si	5.771150000	1.098880000	2.333390000
Si	5.758620000	4.944780000	2.319430000
Si	1.885270000	3.005550000	3.528340000
Si	1.884820000	6.882030000	3.517900000
Si	5.770030000	3.024210000	3.745180000
Si	5.773290000	6.849830000	3.740170000
Si	0.084360000	3.074390000	5.030310000
Si	0.085600000	6.769300000	5.023390000
Si	3.746350000	2.945740000	5.022540000
Si	3.743500000	6.874860000	4.996810000
Si	0.621850000	1.068280000	6.158990000
Si	0.517210000	4.923090000	6.493920000
Si	3.047400000	1.044420000	6.249890000
Si	2.726790000	4.911410000	5.765050000
Cl	7.594060000	1.062520000	8.117620000
Cl	4.339880000	7.264080000	8.658560000

intra dimer tetra-σ_{II} (E = -163.200322 eV)

C	1.910580000	1.010670000	7.506880000
C	1.912080000	0.784060000	8.821690000
H	0.984400000	0.678220000	9.387650000
H	2.843060000	0.682440000	9.383720000
H	0.000000000	0.000000000	0.000000000
H	0.000000000	2.280000000	0.000000000
H	0.000000000	3.847000000	0.000000000
H	0.000000000	6.127000000	0.000000000
H	3.847000000	0.000000000	0.000000000
H	3.847000000	2.280000000	0.000000000
H	3.847000000	3.847000000	0.000000000
H	3.847000000	6.127000000	0.000000000
Si	0.000000000	1.140000000	0.930000000
Si	0.000000000	4.987000000	0.930000000
Si	3.847000000	1.140000000	0.930000000
Si	3.847000000	4.987000000	0.930000000
Si	1.923120000	1.085440000	2.235880000
Si	1.922860000	4.937940000	2.177950000
Si	5.766190000	1.090550000	2.324280000
Si	5.767870000	4.938250000	2.307780000
Si	1.914460000	3.039900000	3.514720000
Si	1.916590000	6.816690000	3.533410000

Si	5.757520000	3.018320000	3.725210000
Si	5.755280000	6.837170000	3.727240000
Si	0.081410000	3.021310000	4.983960000
Si	0.072650000	6.791160000	4.993610000
Si	3.739300000	3.028660000	4.993880000
Si	3.748210000	6.787650000	5.009070000
Si	0.707820000	1.057620000	6.070390000
Si	0.682390000	4.897700000	6.249290000
Si	3.105850000	1.061170000	6.067610000
Si	3.105260000	4.897880000	6.262890000
Cl	7.595360000	4.845880000	8.178940000
Cl	3.803870000	4.839560000	8.223370000

di-σ (I_I) (E = -160.412511 eV)

C	2.672140000	4.964810000	8.055730000
C	1.119040000	4.940540000	8.061530000
H	0.713040000	5.812350000	8.586960000
H	0.745140000	4.034040000	8.552700000
H	0.000000000	0.000000000	0.000000000
H	0.000000000	2.280000000	0.000000000
H	0.000000000	3.847000000	0.000000000
H	0.000000000	6.127000000	0.000000000
H	3.847000000	0.000000000	0.000000000
H	3.847000000	2.280000000	0.000000000
H	3.847000000	3.847000000	0.000000000
H	3.847000000	6.127000000	0.000000000
H	0.000000000	7.701000000	0.000000000
H	0.000000000	9.981000000	0.000000000
H	3.847000000	7.701000000	0.000000000
H	3.847000000	9.981000000	0.000000000
H	0.000000000	11.548000000	0.000000000
H	0.000000000	13.828000000	0.000000000
H	3.847000000	11.548000000	0.000000000
H	3.847000000	13.828000000	0.000000000
Si	0.000000000	1.140000000	0.930000000
Si	0.000000000	4.987000000	0.930000000
Si	3.847000000	1.140000000	0.930000000
Si	3.847000000	4.987000000	0.930000000
Si	0.000000000	8.820000000	0.930000000
Si	0.000000000	12.667000000	0.930000000
Si	3.847000000	8.820000000	0.930000000
Si	3.847000000	12.667000000	0.930000000
Si	1.921890000	1.131070000	2.212430000

Si	1.930660000	4.965860000	2.209990000
Si	5.767650000	1.106020000	2.326340000
Si	5.781830000	4.963350000	2.339950000
Si	1.918670000	3.046520000	3.544820000
Si	1.918790000	6.876210000	3.548090000
Si	5.828590000	3.014420000	3.739480000
Si	5.829920000	6.904850000	3.739480000
Si	0.125300000	2.938670000	5.060480000
Si	0.124630000	6.970050000	5.063980000
Si	3.814050000	3.029930000	5.001580000
Si	3.817490000	6.876440000	5.001990000
Si	0.594320000	1.102630000	6.534380000
Si	0.696820000	4.953040000	6.155560000
Si	2.815280000	1.061320000	5.779520000
Si	3.055980000	4.954170000	6.113530000
Si	1.920450000	8.798640000	2.217010000
Si	5.767180000	8.820170000	2.327500000
Si	1.935760000	10.730540000	3.540350000
Si	5.780470000	10.730320000	3.769640000
Si	0.104550000	10.618320000	5.060100000
Si	3.766340000	10.851110000	5.067240000
Si	0.597100000	8.802840000	6.537800000
Si	2.818710000	8.839950000	5.783610000
Si	1.935390000	12.654760000	2.206340000
Si	5.779550000	12.651870000	2.341910000
Si	1.933960000	14.582390000	3.530000000
Si	5.779430000	14.574750000	3.762720000
Si	0.105450000	14.679650000	5.049580000
Si	3.764060000	14.442570000	5.059070000
Si	1.017510000	12.648890000	5.779260000
Si	3.249090000	12.650600000	6.560620000
Cl	3.308520000	6.460840000	8.862230000
Cl	3.357490000	3.520130000	8.905850000

intra dimer tetra-σ_I (E = -292.206039 eV)

C	1.919290000	4.879360000	7.520020000
C	1.910660000	4.637730000	8.834260000
H	0.980720000	4.530620000	9.397360000
H	2.836820000	4.526970000	9.403080000
H	0.000000000	0.000000000	0.000000000
H	0.000000000	2.280000000	0.000000000
H	0.000000000	3.847000000	0.000000000
H	0.000000000	6.127000000	0.000000000
H	3.847000000	0.000000000	0.000000000

H	3.847000000	2.280000000	0.000000000
H	3.847000000	3.847000000	0.000000000
H	3.847000000	6.127000000	0.000000000
H	0.000000000	7.701000000	0.000000000
H	0.000000000	9.981000000	0.000000000
H	3.847000000	7.701000000	0.000000000
H	3.847000000	9.981000000	0.000000000
H	0.000000000	11.548000000	0.000000000
H	0.000000000	13.828000000	0.000000000
H	3.847000000	11.548000000	0.000000000
H	3.847000000	13.828000000	0.000000000
Si	0.000000000	1.140000000	0.930000000
Si	0.000000000	4.987000000	0.930000000
Si	3.847000000	1.140000000	0.930000000
Si	3.847000000	4.987000000	0.930000000
Si	0.000000000	8.820000000	0.930000000
Si	0.000000000	12.667000000	0.930000000
Si	3.847000000	8.820000000	0.930000000
Si	3.847000000	12.667000000	0.930000000
Si	1.916660000	1.117100000	2.206100000
Si	1.925200000	4.971780000	2.247520000
Si	5.766260000	1.111930000	2.325740000
Si	5.772310000	4.972150000	2.334690000
Si	1.927420000	3.014870000	3.555950000
Si	1.926160000	6.919930000	3.561650000
Si	5.767720000	3.028630000	3.732530000
Si	5.767770000	6.899130000	3.750900000
Si	0.070370000	2.974590000	5.026870000
Si	0.078470000	6.945990000	5.043520000
Si	3.767870000	2.981330000	5.026050000
Si	3.759140000	6.938390000	5.040720000
Si	0.745930000	1.088680000	6.237950000
Si	0.683370000	4.953000000	6.100790000
Si	3.153500000	1.054630000	6.232560000
Si	3.126120000	4.952020000	6.096380000
Si	1.916160000	8.818750000	2.208290000
Si	5.766210000	8.818590000	2.333150000
Si	1.946310000	10.724810000	3.553990000
Si	5.735910000	10.744430000	3.753470000
Si	0.055600000	10.686540000	5.022620000
Si	3.738830000	10.830440000	5.063510000
Si	0.744760000	8.834200000	6.257070000
Si	3.151900000	8.868580000	6.243990000
Si	1.926730000	12.659420000	2.225820000

Si	5.772950000	12.657850000	2.326410000
Si	1.945850000	14.595950000	3.548530000
Si	5.734920000	14.572150000	3.747660000
Si	0.054640000	14.618880000	5.015940000
Si	3.738300000	14.480240000	5.057440000
Si	1.060560000	12.653630000	5.767340000
Si	3.279950000	12.657760000	6.528330000
Cl	3.890220000	8.844530000	8.202670000
Cl	3.891120000	1.064610000	8.193980000

end-bridge ($I_{I'}$) （E = -289.773030 eV）

C	8.114040000	3.792150000	7.866490000
C	7.745900000	2.290440000	7.791050000
H	6.656440000	2.218870000	7.653580000
H	7.989750000	1.818990000	8.753030000
H	7.694000000	0.000000000	0.000000000
H	7.694000000	2.280000000	0.000000000
H	7.694000000	3.847000000	0.000000000
H	7.694000000	6.127000000	0.000000000
H	11.541000000	0.000000000	0.000000000
H	11.541000000	2.280000000	0.000000000
H	11.541000000	3.847000000	0.000000000
H	11.541000000	6.127000000	0.000000000
H	0.000000000	0.000000000	0.000000000
H	0.000000000	2.280000000	0.000000000
H	0.000000000	3.847000000	0.000000000
H	0.000000000	6.127000000	0.000000000
H	3.847000000	0.000000000	0.000000000
H	3.847000000	2.280000000	0.000000000
H	3.847000000	3.847000000	0.000000000
H	3.847000000	6.127000000	0.000000000
Si	7.694000000	1.140000000	0.930000000
Si	7.694000000	4.987000000	0.930000000
Si	11.541000000	1.140000000	0.930000000
Si	11.541000000	4.987000000	0.930000000
Si	0.000000000	1.140000000	0.930000000
Si	0.000000000	4.987000000	0.930000000
Si	3.847000000	1.140000000	0.930000000
Si	3.847000000	4.987000000	0.930000000
Si	9.624380000	1.050340000	2.228710000
Si	9.614010000	5.004450000	2.206740000
Si	13.478090000	1.115800000	2.331910000
Si	13.459520000	4.969410000	2.332070000

Si	9.680260000	3.040250000	3.421210000
Si	9.551250000	6.842840000	3.682280000
Si	13.489630000	3.038550000	3.736290000
Si	13.461880000	6.885910000	3.763700000
Si	7.791120000	2.982690000	4.737800000
Si	7.726050000	6.942320000	5.268120000
Si	11.475080000	2.890130000	4.984060000
Si	11.468090000	7.013740000	5.098540000
Si	8.522750000	1.340090000	6.266010000
Si	8.346540000	4.761530000	6.139930000
Si	10.948300000	1.159750000	6.544500000
Si	10.702040000	4.929490000	5.771790000
Si	1.932040000	1.121810000	2.204700000
Si	1.915000000	4.966270000	2.205080000
Si	5.763470000	1.090020000	2.314030000
Si	5.759830000	4.993510000	2.338600000
Si	1.924390000	3.041440000	3.535150000
Si	1.914950000	6.889300000	3.529770000
Si	5.711050000	3.023800000	3.668310000
Si	5.777540000	6.901530000	3.812120000
Si	0.097460000	3.143550000	5.051940000
Si	0.089940000	6.765900000	5.054660000
Si	3.756270000	2.909030000	5.049690000
Si	3.737720000	6.994270000	5.045930000
Si	0.998630000	1.105720000	5.777680000
Si	0.622140000	4.952940000	6.540810000
Si	3.234750000	1.102650000	6.546860000
Si	2.853960000	4.949590000	5.767650000
Cl	6.833430000	4.665310000	8.830840000
Cl	9.701670000	3.954440000	8.761020000

inter dimer tetra-σ_I (E = -291.667115 eV)

C	8.248450000	2.984620000	7.542600000
C	8.200680000	2.955920000	8.879600000
H	8.187730000	2.020390000	9.443010000
H	8.176450000	3.870770000	9.474380000
H	7.694000000	0.000000000	0.000000000
H	7.694000000	2.280000000	0.000000000
H	7.694000000	3.847000000	0.000000000
H	7.694000000	6.127000000	0.000000000
H	11.541000000	0.000000000	0.000000000
H	11.541000000	2.280000000	0.000000000
H	11.541000000	3.847000000	0.000000000
H	11.541000000	6.127000000	0.000000000

H	0.000000000	0.000000000	0.000000000
H	0.000000000	2.280000000	0.000000000
H	0.000000000	3.847000000	0.000000000
H	0.000000000	6.127000000	0.000000000
H	3.847000000	0.000000000	0.000000000
H	3.847000000	2.280000000	0.000000000
H	3.847000000	3.847000000	0.000000000
H	3.847000000	6.127000000	0.000000000
Si	7.694000000	1.140000000	0.930000000
Si	7.694000000	4.987000000	0.930000000
Si	11.541000000	1.140000000	0.930000000
Si	11.541000000	4.987000000	0.930000000
Si	0.000000000	1.140000000	0.930000000
Si	0.000000000	4.987000000	0.930000000
Si	3.847000000	1.140000000	0.930000000
Si	3.847000000	4.987000000	0.930000000
Si	9.618800000	1.054110000	2.217940000
Si	9.619110000	5.042600000	2.222860000
Si	13.473450000	1.105310000	2.324880000
Si	13.468830000	4.965070000	2.312020000
Si	9.708500000	3.044010000	3.387050000
Si	9.502400000	6.907270000	3.724990000
Si	13.561860000	3.036530000	3.703240000
Si	13.502140000	6.868460000	3.747860000
Si	7.776460000	3.031660000	4.622580000
Si	7.701880000	6.856790000	5.401830000
Si	11.540770000	3.043080000	4.911280000
Si	11.480870000	6.803430000	5.039590000
Si	8.362920000	1.472200000	6.263730000
Si	8.397840000	4.526750000	6.295550000
Si	10.692870000	1.123820000	5.878730000
Si	10.792410000	4.854130000	6.216890000
Si	1.929610000	1.117720000	2.225880000
Si	1.916290000	4.959560000	2.207150000
Si	5.768160000	1.075090000	2.327010000
Si	5.760300000	5.004090000	2.336770000
Si	1.959170000	3.045190000	3.541920000
Si	1.940030000	6.872450000	3.535470000
Si	5.666540000	3.031300000	3.644620000
Si	5.766850000	6.884640000	3.858390000
Si	0.131100000	3.134870000	5.053410000
Si	0.111280000	6.748020000	5.058380000
Si	3.742770000	2.971590000	5.058700000
Si	3.714920000	6.924970000	5.058130000

Si	1.024430000	1.091690000	5.741230000
Si	0.689930000	4.938880000	6.487590000
Si	3.245870000	1.100320000	6.453860000
Si	3.122660000	4.944910000	6.216720000
Cl	4.009120000	4.933240000	8.128660000
Cl	11.560280000	4.851880000	8.163890000

inter dimer tetra-σ_{II} (E = -162.721577 eV)

C	3.307830000	3.011110000	7.517700000
C	3.376850000	2.997760000	8.853460000
H	3.399810000	2.066000000	9.421940000
H	3.403030000	3.917230000	9.441050000
H	0.000000000	0.000000000	0.000000000
H	0.000000000	2.280000000	0.000000000
H	0.000000000	3.847000000	0.000000000
H	0.000000000	6.127000000	0.000000000
H	3.847000000	0.000000000	0.000000000
H	3.847000000	2.280000000	0.000000000
H	3.847000000	3.847000000	0.000000000
H	3.847000000	6.127000000	0.000000000
Si	0.000000000	1.140000000	0.930000000
Si	0.000000000	4.987000000	0.930000000
Si	3.847000000	1.140000000	0.930000000
Si	3.847000000	4.987000000	0.930000000
Si	1.921340000	1.048770000	2.214300000
Si	1.921160000	5.030050000	2.214470000
Si	5.770730000	1.069570000	2.318880000
Si	5.769900000	5.013790000	2.320090000
Si	1.779140000	3.037180000	3.374950000
Si	2.035770000	6.881550000	3.688750000
Si	5.776880000	3.037610000	3.603220000
Si	5.744670000	6.883220000	3.854760000
Si	0.019920000	3.026010000	4.953500000
Si	0.126320000	6.869310000	5.038940000
Si	3.692790000	3.026380000	4.615840000
Si	3.807310000	6.872380000	5.394420000
Si	0.713080000	1.145150000	6.194380000
Si	0.717500000	4.895870000	6.200480000
Si	3.109100000	1.490160000	6.264380000
Si	3.112890000	4.546420000	6.275790000
Cl	-0.049770000	4.890550000	8.144930000
Cl	-0.046140000	1.130460000	8.141750000

[3] Imaginary vibrational frequencies of the transition states along single and double dechlorination processes of *trans* and iso-DCE dissociation on Si(100) are shown in Figure S1 and S2

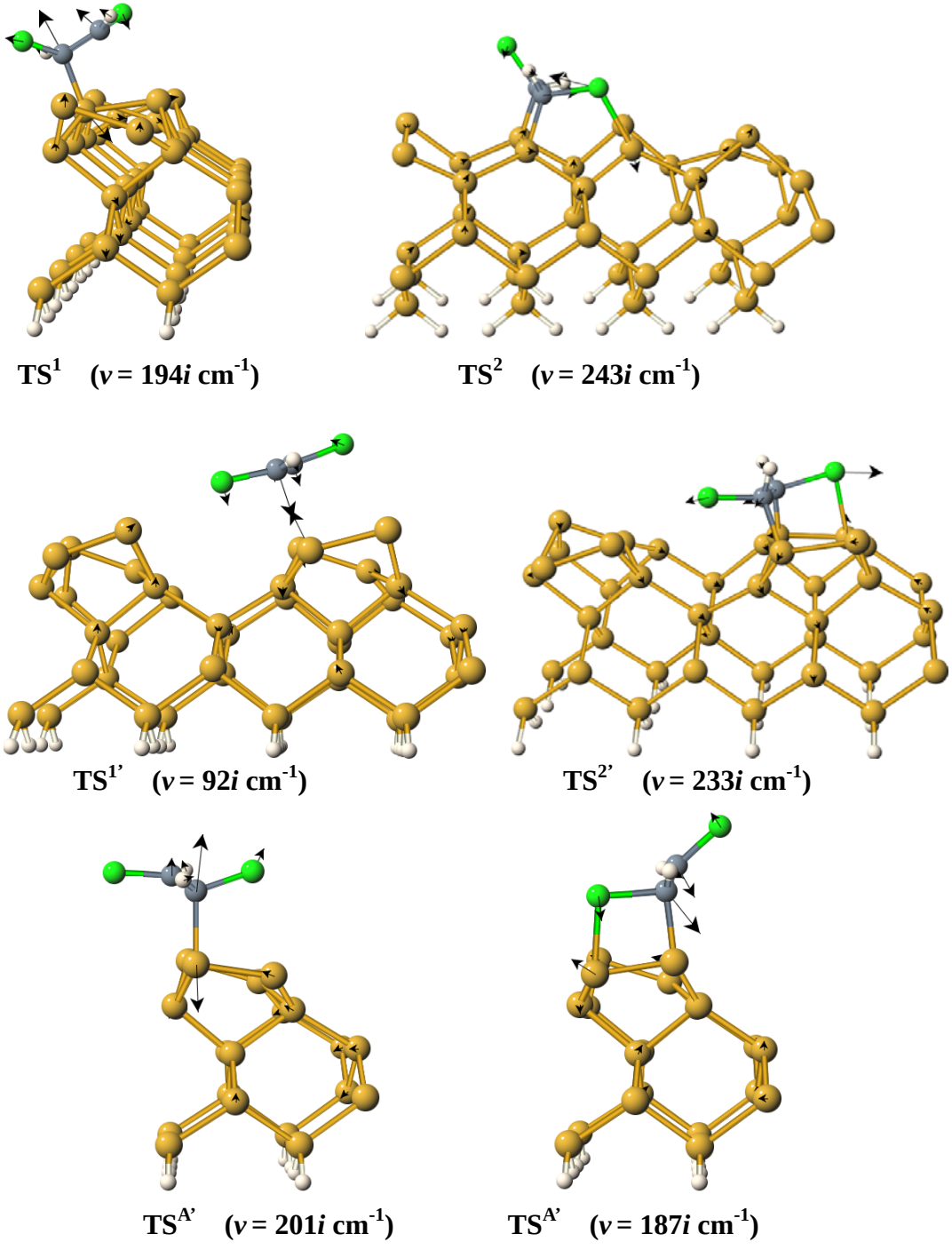
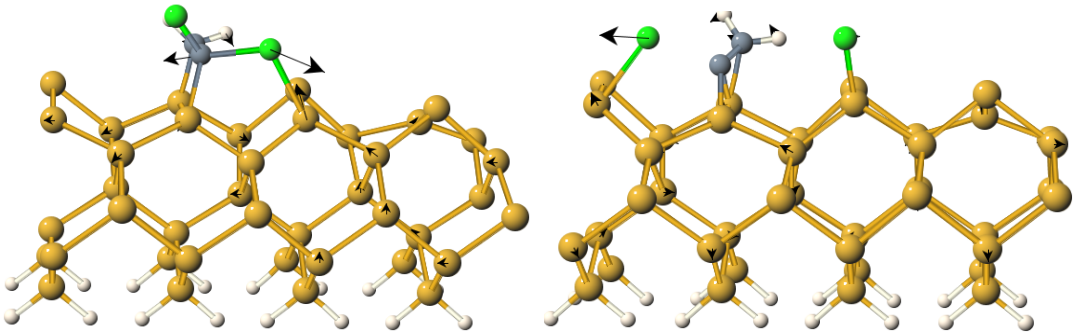
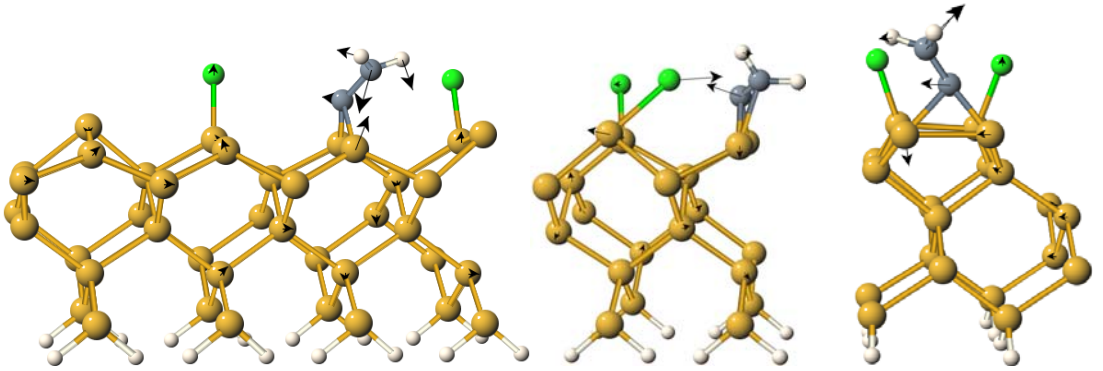


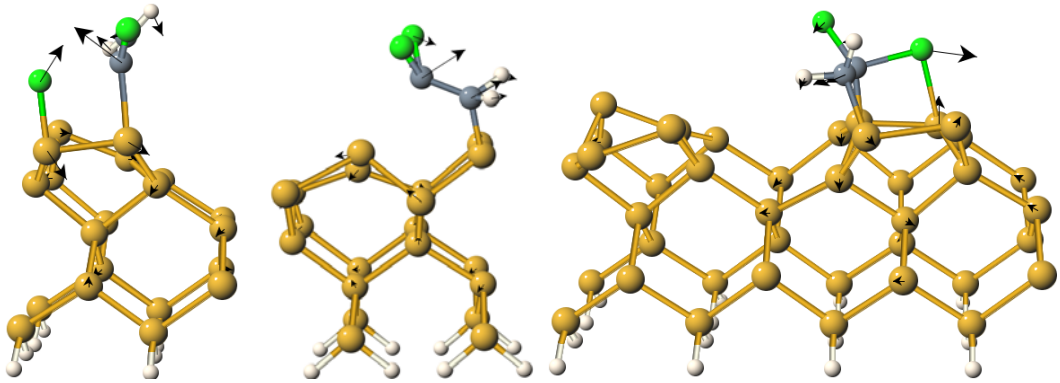
Figure S1 The vibrational mode of imaginary frequency in each transition state along the reaction pathways of *trans*-DCE dechlorination on Si(100) plotted in Figure 2.



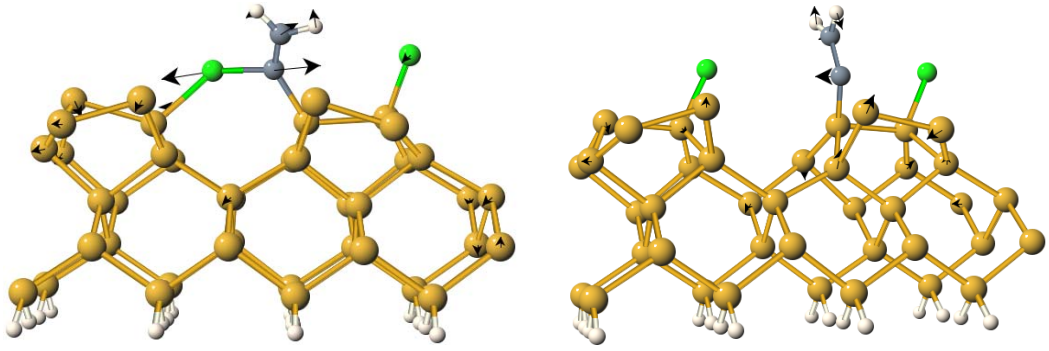
TS_I^1 (ν = 214*i* cm^{-1}) TS_I^2 (ν = 45*i* cm^{-1})



TS_I^3 (ν = 284*i* cm^{-1}) TS_{II}^2 (ν = 276*i* cm^{-1}) TS_{II}^2 (ν = 303*i* cm^{-1})



TS^{up} (ν = 294*i* cm^{-1}) $TS_{I'}$ (ν = 127*i* cm^{-1}) $TS_{I'}^1$ (ν = 198*i* cm^{-1})



$TS_{I'}^2$ (ν = 229*i* cm^{-1}) $TS_{I'}^3$ (ν = 154*i* cm^{-1})

Figure S2 The vibrational mode of imaginary frequency in each transition state along the reaction pathways I, II and I' of *iso*-DCE dechlorination on Si(100) plotted in Figures 4 and 5.