

Electron Transport through Cyclic Disulfide Molecular Junctions with Two Adsorption States at the Contact: a Density Functional Theory Study

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Supporting Information

Table S1. DZP Basis set used for Au in the periodic DFT calculations.

```

number of radial functions [5d/5d/6s/6s/6p]
5
angular momentum, number of alphas
0 4
alphas - s
0.0910595 0.2350206 0.7910678 1.4150629
wave function coefficients
0.2346158 0.3412113 -1.1978413 0.6566866
angular momentum, number of alphas
0 1
alphas - s - DZ
0.0910595
wave function coefficients
1.00000000d+00
angular momentum, number of alphas
1 2
alphas - p
0.1319557 0.2817063
wave function coefficients
0.382936 -0.3004869
angular momentum, number of alphas
2 5
alphas - d
0.1156919 0.2904125 0.6459106 1.4727935 5.2071920
wave function coefficients
0.0067081 0.0880612 0.4798959 2.0655605 -0.1721454
angular momentum, number of alphas
2 1
alphas - d - DZ
0.1156919
wave function coefficients
1.0000000

```

Table S2. SZP Basis set used for Au in the periodic DFT calculations.

```

number of radial functions [5d/6s/6p]
3
angular momentum, number of alphas
0 3
alphas - s
0.1104004 0.9508066 1.8802514
wave function coefficients
0.4067879 -0.8810795 0.5207425
angular momentum, number of alphas
1 2
alphas - p
0.1319557 0.2817063
wave function coefficients
0.382936 -0.3004869
angular momentum, number of alphas
2 5
alphas - d -
0.1256919 0.2904125 0.6459106 1.4727935 5.2071920
wave function coefficients
0.0057081 0.0880612 0.4798959 2.0655605 -0.1721454

```

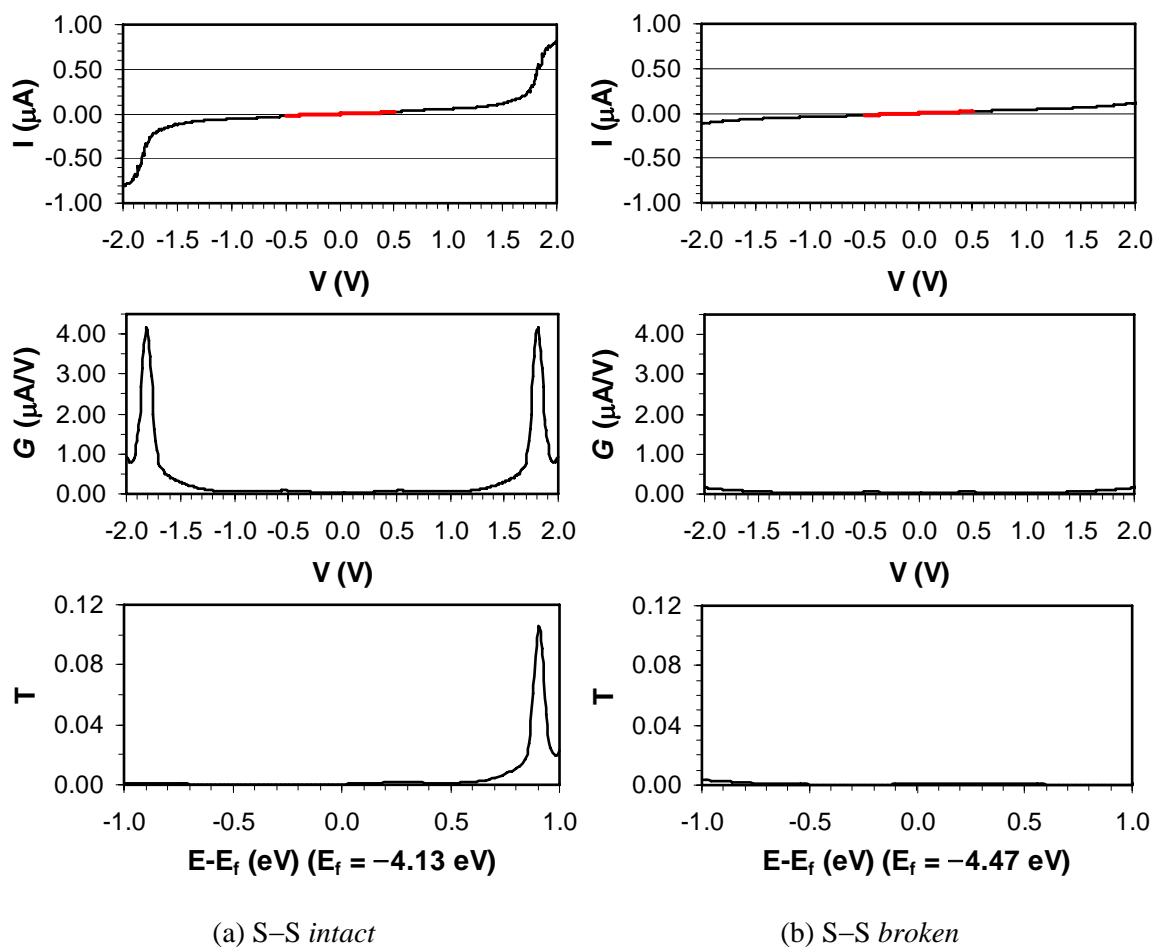


Figure S1. I - V (current-voltage), G - V (conductance-voltage where the conductance $G = dI/dV$), and $T(E)$ (transmission) curves of the model junction devices of cyclic (a) and acyclic (b) 1,2-dithiolanes.