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

Yun Hee Jang[††] and William A. Goddard, III[*,†]

Materials and Process Simulation Center (139-74), California Institute of Technology, Pasadena, California 91125; Department of Materials Science and Engineering, Gwangju Institute of Science and Technology, Gwangju 500-712, Korea; LEMA, Université François Rabelais, 37200 Tours, France.

[*]*To whom correspondence should be sent (Phone 626-395-2731, Fax 626-585-0918, E-mail wag@wag.caltech.edu)*

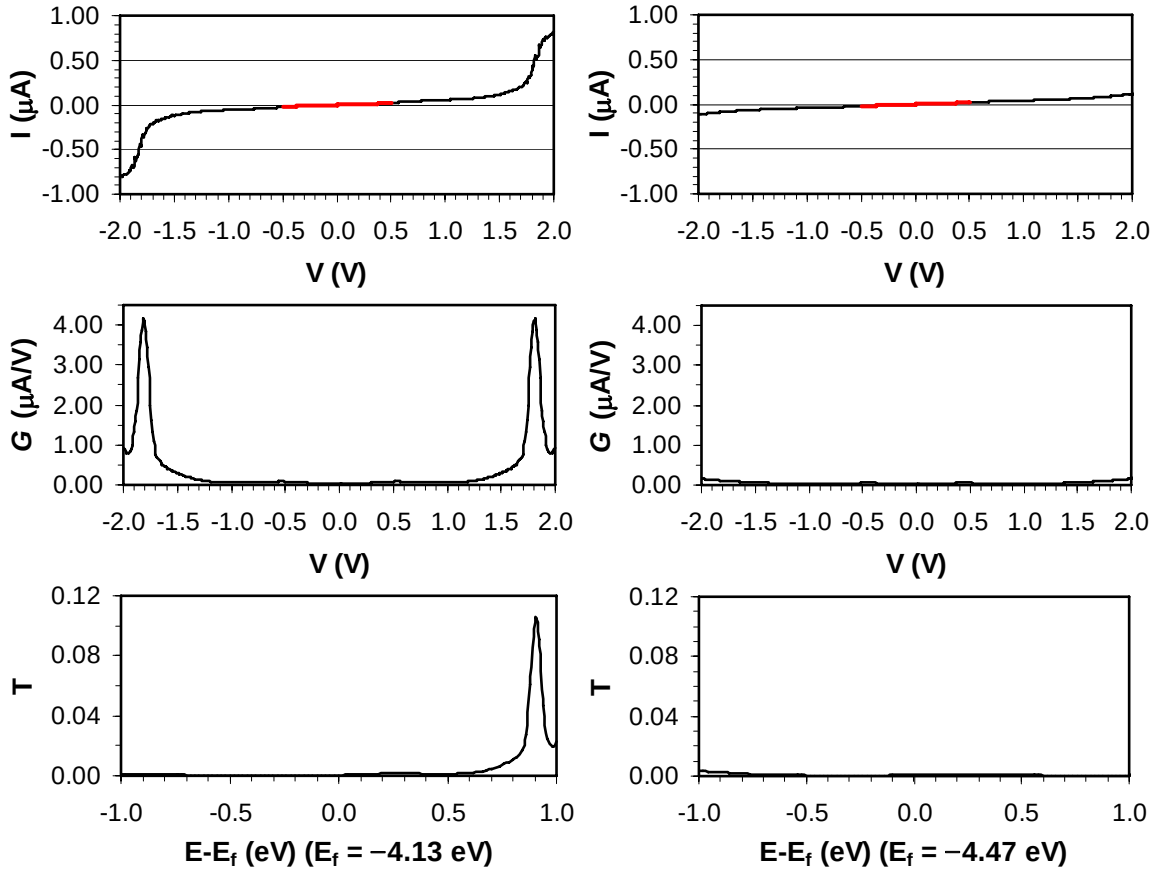
Supporting Information

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
```



(a) S–S *intact* (b) S–S *broken*

Figure S1. *I–V* (current–voltage), *G–V* (conductance–voltage where the conductance $G = \mathrm{d}I/\mathrm{d}V$), and $T(E)$ (transmission) curves of the model junction devices of *cyclic* (a) and *acyclic* (b) 1,2-dithiolanes.