Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Molecular Quantum Cellular Automata Cell Design Trade-offs: Latching vs Power Dissipation

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Electronic Supporting Information

UHF/STO-3G Cs charge localized local minimum

6	-0.003372	-3.857163	1.230307
1	0.211755	-3.374890	2.173578
1	-0.421984	-4.853210	1.265525
6	0.268260	-3.225081	0.000000
6	-0.003372	-3.857163	-1.230307
1	-0.421984	-4.853210	-1.265525
1	0.211755	-3.374890	-2.173578
6	0.841045	-1.801261	0.000000
1	1.468000	-1.657766	0.877715
1	1.468000	-1.657766	-0.877715
6	-0.279273	-0.731554	0.000000
1	-0.909788	-0.864577	0.877128
1	-0.909788	-0.864577	-0.877128
6	0.294604	0.703128	0.000000
1	0.922295	0.848153	-0.877854
1	0.922295	0.848153	0.877854
6	-0.836004	1.765467	0.000000
1	-1.465367	1.638497	0.878833
1	-1.465367	1.638497	-0.878833
6	-0.283291	3.197721	0.000000
6	-0.003372	3.888507	-1.171206
1	0.409759	4.906171	-1.166319
1	-0.190229	3.444289	-2.159279
6	-0.003372	3.888507	1.171206
1	0.409759	4.906171	1.166319
1	-0.190229	3.444289	2.159279

```
#P scf/sto-3g freq
Full point group                 CS      NOp   2
SCF Done:  E(UHF) =  -383.053634847     A.U. after   18 cycles
Frequencies --     23.5674                38.5068                40.7991
Sum of electronic and thermal Free Energies=         -382.828103
```

UHF/STO-3G C2h charge delocalized local minimum

6	-1.443100	3.587170	1.198493
1	-1.456452	3.083123	2.163130
1	-1.431973	4.675584	1.212423
6	-1.452042	2.874459	0.000000
6	-1.443100	3.587170	-1.198493
1	-1.431973	4.675584	-1.212423
1	-1.456452	3.083123	-2.163130
6	-1.443100	1.341083	0.000000
1	-1.976060	0.981778	0.877961
1	-1.976060	0.981778	-0.877961
6	-0.002228	0.771997	0.000000
1	0.529909	1.136502	0.877141
1	0.529909	1.136502	-0.877141
6	0.002228	-0.771997	0.000000
1	-0.529909	-1.136502	-0.877141
1	-0.529909	-1.136502	0.877141
6	1.443100	-1.341083	0.000000

```
 1    1.976060   -0.981778    0.877961
 1    1.976060   -0.981778   -0.877961
 6    1.452042   -2.874459    0.000000
 6    1.443100   -3.587170   -1.198493
 1    1.431973   -4.675584   -1.212423
 1    1.456452   -3.083123   -2.163130
 6    1.443100   -3.587170    1.198493
 1    1.431973   -4.675584    1.212423
 1    1.456452   -3.083123    2.163130

#P scf/sto-3g freq
Full point group                 C2H     NOp   4
SCF Done:  E(UHF) =  -383.013362444     A.U. after   16 cycles
Frequencies --     23.0245                37.9791                39.1082
Sum of electronic and thermal Free Energies=         -382.786713
```

CASSCF(1,2)/6-31G* C1 charge localized and twisted local minimum

```
      6         3.969257   -1.123166   -0.077238
      1         3.635791   -2.109066    0.192849
      1         4.949311   -1.050481   -0.513098
      6         3.214538   -0.043159    0.126588
      6         3.676062    1.277978   -0.227704
      1         4.639335    1.418033   -0.677703
      1         3.101041    2.153992    0.004259
      6         1.827880   -0.162110    0.728962
      1         1.713965   -1.142541    1.180075
      1         1.718447    0.566014    1.529776
      6         0.715271    0.051491   -0.306220
      1         0.827148   -0.681653   -1.100531
      1         0.826168    1.028122   -0.769589
      6        -0.682442   -0.063885    0.305449
      1        -0.798717    0.671381    1.099198
      1        -0.799092   -1.040192    0.771820
      6        -1.790475    0.135919   -0.741272
      1        -1.686436   -0.594113   -1.536459
      1        -1.692621    1.111094   -1.205552
      6        -3.179873    0.014728   -0.144038
      6        -3.873974    1.088560    0.367274
      1        -4.848401    0.977298    0.807831
      1        -3.470318    2.085927    0.340248
      6        -3.852526   -1.183314   -0.048147
      1        -4.827322   -1.253119    0.400030
      1        -3.430605   -2.098948   -0.425072

#P cas(1,2)/6-31G* freq
Full point group                 C1      NOp   1
  ( 1)     EIGENVALUE    -387.6315185988
Frequencies --    279.1857               329.1523               386.4387
Sum of electronic and thermal Free Energies=         -387.206503
```

CASSCF(1,2)/STO-3G Cs charge localized local minimum

```
      6         0.000783    3.826337    1.199117
      1        -0.220342    3.357446    2.140337
      1         0.424957    4.812271    1.233725
      6        -0.261850    3.206581   -0.000000
      6         0.000783    3.826337   -1.199117
      1         0.424957    4.812271   -1.233725
      1        -0.220342    3.357446   -2.140337
      6        -0.827924    1.795153   -0.000000
      1        -1.462037    1.658411    0.871068
      1        -1.462037    1.658411   -0.871068
      6         0.274390    0.728121   -0.000000
      1         0.909322    0.868873    0.870779
      1         0.909322    0.868873   -0.870779
      6        -0.286279   -0.695656    0.000000
```

```
      1        -0.921975   -0.840437   -0.871396
      1        -0.921975   -0.840437    0.871396
      6         0.827223   -1.755513    0.000000
      1         1.463694   -1.626161    0.868585
      1         1.463694   -1.626161   -0.868585
      6         0.280057   -3.170608    0.000000
      6         0.000783   -3.867434   -1.154610
      1        -0.408433   -4.861544   -1.133062
      1         0.188569   -3.446508   -2.127347
      6         0.000783   -3.867434    1.154610
      1        -0.408433   -4.861544    1.133062
      1         0.188569   -3.446508    2.127347

 #P cas(1,2)/6-31G* freq
 Full point group                 CS      NOp   2
   ( 1)     EIGENVALUE    -387.6277002562
 Frequencies --    286.6997               328.5673               590.8918
 Sum of electronic and thermal Free Energies=         -386.526167
```

CASSCF(1,2)/6-31G* C2h geometry but broken symmetry wavefunction results

```
  6   0.0000000   3.8468855   1.1768635
  1  -0.2044555   3.4019770   2.1338420
  1   0.4166950   4.8369075   1.1833935
  6  -0.2709535   3.1885945   0.0000000
  6   0.0000000   3.8468855  -1.1768635
  1   0.4166950   4.8369075  -1.1833935
  1  -0.2044555   3.4019770  -2.1338420
  6  -0.8275735   1.7753330   0.0000000
  1  -1.4628655   1.6422860   0.8698265
  1  -1.4628655   1.6422860  -0.8698265
  6   0.2803345   0.7118885   0.0000000
  1   0.9156485   0.8546550   0.8710875
  1   0.9156485   0.8546550  -0.8710875
  6  -0.2803345  -0.7118885   0.0000000
  1  -0.9156485  -0.8546550  -0.8710875
  1  -0.9156485  -0.8546550   0.8710875
  6   0.8275735  -1.7753330   0.0000000
  1   1.4628655  -1.6422860   0.8698265
  1   1.4628655  -1.6422860  -0.8698265
  6   0.2709535  -3.1885945   0.0000000
  6   0.0000000  -3.8468855  -1.1768635
  1  -0.4166950  -4.8369075  -1.1833935
  1   0.2044555  -3.4019770  -2.1338420
  6   0.0000000  -3.8468855   1.1768635
  1  -0.4166950  -4.8369075   1.1833935
  1   0.2044555  -3.4019770   2.1338420

   ( 1)     EIGENVALUE    -387.6261300864
```

B3LYP/6-31G* C2h minimum

```
  6   -1.436423    3.577997    1.191285
  1   -1.461890    3.079807    2.156339
  1   -1.415702    4.663987    1.198473
  6   -1.443901    2.863651    0.000000
  6   -1.436423    3.577997   -1.191285
  1   -1.415702    4.663987   -1.198473
  1   -1.461890    3.079807   -2.156339
  6   -1.436423    1.345134    0.000000
  1   -1.980593    0.979771    0.878938
  1   -1.980593    0.979771   -0.878938
  6   -0.006813    0.766652    0.000000
  1    0.536607    1.142156    0.878325
  1    0.536607    1.142156   -0.878325
  6    0.006813   -0.766652    0.000000
```

```
 1   -0.536607   -1.142156   -0.878325
 1   -0.536607   -1.142156    0.878325
 6    1.436423   -1.345134    0.000000
 1    1.980593   -0.979771    0.878938
 1    1.980593   -0.979771   -0.878938
 6    1.443901   -2.863651    0.000000
 6    1.436423   -3.577997   -1.191285
 1    1.415702   -4.663987   -1.198473
 1    1.461890   -3.079807   -2.156339
 6    1.436423   -3.577997    1.191285
 1    1.415702   -4.663987    1.198473
 1    1.461890   -3.079807    2.156339

#P b3lyp/6-31G* freq
Full point group                 C2H     NOp   4
SCF Done:  E(UB3LYP) =  -390.329687083     A.U. after   15 cycles
Frequencies --     26.0787               37.4941               39.7178
Sum of electroni
```