Exploring the spatial features of electronic transitions in molecular and biomolecular systems by swift electrons

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Numerical integration procedure of the OAM-EELS rate

The numerical integration of the energy loss rate per unit of angular momentum, eq(10), imply the discretization of the molecular transition potential $V_{0n}(r)$. Due to the dimension of the large systems treated, we use a linear response TD-DFT approach:¹ indeed, the optimal compromise between accuracy and computational cost makes TD-DFT the most widely used method of calculating excitation energies of chemically relevant systems.

Figure 1: cube grid centered on a G-quadruplex
The transition potential is therefore expressed as:

\[
V_{0n}(\mathbf{r}) = \int d\mathbf{r}' \frac{\rho(\mathbf{r}', \omega_{0n})}{|\mathbf{r} - \mathbf{r}'|} = \sum_{ia} \int d\mathbf{r}' \left[ \phi_{i}(\mathbf{r}') \phi_{a}^{*}(\mathbf{r}') X_{ia}(\omega_{0n}) + \phi_{a}(\mathbf{r}') \phi_{i}^{*}(\mathbf{r}') Y_{ia}(\omega_{0n}) \right] \frac{1}{|\mathbf{r} - \mathbf{r}'|} \]

(1)

\(X_{ia}(\omega_{0n})\) and \(Y_{ia}(\omega_{0n})\) refer to the excitation and de-excitation coefficients involving all the possible pair of occupied \(\phi_{i}(\mathbf{r}')\) and virtual \(\phi_{a}(\mathbf{r}')\) orbitals that describe a transition from the ground (\(|0\rangle\)) to an excited state (\(|n\rangle\)) associated to an energy difference of \(\omega_{0n}\). The quantity in eq.(1) have been discretized over a cubic grid (with a length side of \(L\), fig.1) by slightly modifying the input of the G16 software,\(^2\) and then averaged along the direction \(p = k_{z,f} - k_{z,i}\):

\[
\tilde{V}_{p}^{0n}(\mathbf{r}_{\perp}) = V_{0n}(x,y,p) = \frac{1}{L} \sum_{z=-L/2}^{L/2} V_{0n}(x,y,z) \cdot e^{-ipz} \]

(2)

The eq.(2) of the manuscript have been finally integrated over the grid cube, by a home-made Matlab script.

**Computational details**

We report in this section the computational details used in the simulations, the geometrical structures, the excitation energies, the oscillator strengths and the final OAM resolved transition probabilities of studied systems.

**Coordinates of the structures**

The coordinates (in Angstrom) of the geometrical structures of different molecular systems are here reported.
Table 1: Coordinates (Angstrom) of the optimized guanine structure.

| Atomic num. | X     | Y     | Z     |
|------------|-------|-------|-------|
| 6          | 0.527396 | -0.848145 | -0.000496 |
| 6          | 0.852889 | 0.503229 | 0.006425 |
| 7          | -0.694082 | -1.431941 | 0.006852 |
| 6          | -1.669670 | -0.564036 | -0.003188 |
| 7          | 2.220761  | 0.676588 | 0.006069 |
| 1          | 3.755825  | -0.784696 | 0.000844 |
| 6          | 2.708797  | -0.530077 | 0.001573 |
| 7          | 1.726856  | -1.501188 | -0.002774 |
| 1          | 1.849904  | -2.499212 | -0.010476 |
| 6          | -0.209959 | 1.468808 | 0.002677 |
| 8          | -0.191592 | 2.680114 | -0.002454 |
| 7          | -1.473623 | 0.787371 | -0.003150 |
| 1          | -2.265157 | 1.410920 | -0.066178 |
| 7          | -2.968795 | -1.004832 | -0.066863 |
| 1          | -3.064106 | -1.992225 | 0.107193 |
| 1          | -3.678270 | -0.436363 | 0.365378 |
Table 2: Coordinates (Angstrom) of the guanine tetramer. The first 16 atoms correspond to the extracted monomer.

| Atomic num. | Guanine tetramer (first part) | Guanine tetramer (second part) |
|-------------|-------------------------------|--------------------------------|
| X           | Y                             | Z                              |
| X           | Y                             | Z                              |
| Atomic num. | X                             | Y                             | Z     |
| 6           | 7.124327                      | 2.025491                      | 3.630807 |
| 6           | 7.815970                      | 3.240532                      | 3.585003 |
| 7           | 5.779680                      | 1.840050                      | 3.646899 |
| 6           | 5.078949                      | 2.987362                      | 3.615867 |
| 7           | 9.188858                      | 3.018085                      | 3.572269 |
| 1           | 10.253991                     | 1.158362                      | 3.607276 |
| 6           | 9.312348                      | 1.696283                      | 3.612156 |
| 7           | 8.092717                      | 1.044264                      | 3.654290 |
| 1           | 5.093909                      | 0.099009                      | 3.547453 |
| 7           | 3.726185                      | 2.927002                      | 3.630253 |
| 1           | 3.304059                      | 2.017258                      | 3.485154 |
| 1           | 3.117740                      | 3.762059                      | 3.543164 |
| 6           | 5.852214                      | 13.716316                     | 3.680861 |
| 6           | 5.161402                      | 12.500891                     | 3.644500 |
| 7           | 7.196996                      | 13.903079                     | 3.682239 |
| 6           | 7.898841                      | 12.756290                     | 3.643754 |
| 7           | 3.788280                      | 12.723837                     | 3.631236 |
| 1           | 2.722884                      | 14.582529                     | 3.654934 |
| 6           | 3.664574                      | 14.045178                     | 3.664321 |
| 7           | 4.884248                      | 14.697496                     | 3.700946 |
| 1           | 5.078446                      | 15.724232                     | 3.693632 |
| 6           | 5.902649                      | 11.279515                     | 3.587592 |
| 8           | 5.472693                      | 10.113603                     | 3.507215 |
| 7           | 7.305081                      | 11.511765                     | 3.608361 |
| 1           | 7.882460                      | 10.646625                     | 3.542254 |
| 7           | 9.250935                      | 12.817400                     | 3.651762 |
| 1           | 9.672655                      | 13.729362                     | 3.519903 |
| 1           | 9.860913                      | 11.983377                     | 3.563293 |
Table 3: Coordinates (Angstrom) of the L-alanine.

| Atomic num. | X          | Y          | Z          |
|-------------|------------|------------|------------|
| 7           | 1.280452   | -1.135863  | 0.238015   |
| 1           | -0.363503  | -1.588108  | -0.623873  |
| 6           | 0.621780   | 0.167930   | 0.423392   |
| 1           | 0.672247   | 0.513619   | 1.458338   |
| 6           | 1.249350   | 1.229605   | -0.479824  |
| 6           | -0.876223  | 0.046556   | 0.088166   |
| 1           | 1.230769   | 0.907089   | -1.522457  |
| 1           | 0.696031   | 2.162401   | -0.398987  |
| 1           | 2.285385   | 1.413109   | -0.191154  |
| 8           | -1.201375  | -1.079117  | -0.561303  |
| 1           | 1.324027   | -1.662055  | 1.101125   |
| 8           | -1.673970  | 0.900814   | 0.364784   |
| 1           | 2.225200   | -1.033135  | -0.107347  |

Table 4: Coordinates (Angstrom) of the D-alanine.

| Atomic num. | X          | Y          | Z          |
|-------------|------------|------------|------------|
| 6           | 0.621864   | -0.167998  | 0.423331   |
| 6           | 1.249342   | -1.229479  | -0.480095  |
| 6           | -0.876217  | -0.046528  | 0.088182   |
| 1           | 0.696051   | -2.162307  | -0.399261  |
| 1           | 1.230606   | -0.906912  | -1.522707  |
| 1           | 2.285426   | -1.413035  | -0.191631  |
| 8           | -1.201354  | 1.078865   | -0.561779  |
| 1           | 0.672170   | -0.513967  | 1.458206   |
| 7           | 1.280547   | 1.135824   | 0.238280   |
| 1           | -0.363487  | 1.587840   | -0.624691  |
| 1           | 1.322755   | 1.662345   | 1.101268   |
| 8           | -1.674042  | -0.900579  | 0.365257   |
| 1           | 2.225884   | 1.033002   | -0.105468  |
Table 5: Coordinates (Angstrom) of Gquadruplex 2MB2. First layer.

| Atomic num. | X     | Y     | Z     | Atomic num. | X     | Y     | Z     |
|-------------|-------|-------|-------|-------------|-------|-------|-------|
| 6           | -3.254354 | -2.520009 | 3.027107 | 6           | -1.145159 | 5.399237 | -3.732626 |
| 1           | -3.615623 | -1.951693 | 2.156515 | 1           | -0.883116 | 6.054751 | -4.577057 |
| 1           | -3.960043 | -2.09807 | 3.939316 | 1           | -0.958827 | 5.940084 | -2.792310 |
| 1           | -3.59108  | -3.571993 | 2.931273 | 1           | -2.208457 | 5.126829 | -3.795233 |
| 7           | -1.804667 | -2.462697 | 3.096973 | 7           | -0.352438 | 4.182943 | -3.777142 |
| 6           | -0.905280 | -3.510106 | 3.055813 | 6           | -0.794386 | 2.878406 | -3.875075 |
| 1           | -1.248047 | -4.541619 | 2.959861 | 1           | -1.859524 | 2.649050 | -3.936924 |
| 7           | 0.366387  | -3.127127 | 3.143061 | 7           | 0.187854  | 1.980425 | -3.895731 |
| 6           | 0.279688  | -1.753096 | 3.246367 | 6           | 1.328116  | 2.752663 | -3.797745 |
| 6           | 1.327627  | -0.760867 | 3.371064 | 6           | 2.720950  | 3.265271 | -3.764128 |
| 8           | 2.543734  | -0.867965 | 3.417564 | 8           | 3.252149  | 1.257151 | -3.812210 |
| 7           | 0.724964  | 0.542113  | 3.445551 | 7           | 3.535398  | 3.354582 | -3.653083 |
| 1           | 1.409075  | 1.291761  | 3.534907 | 1           | 4.532526  | 3.328660 | -3.624804 |
| 6           | -0.617204 | 0.845832  | 3.408707 | 6           | 3.109093  | 4.842947 | -3.587898 |
| 7           | -0.951457 | 2.168681  | 3.496852 | 7           | 4.078294  | 5.801862 | -3.485174 |
| 1           | -0.261798 | 2.899210  | 3.584967 | 1           | 5.061783  | 5.580365 | -3.457685 |
| 1           | -1.933988 | 2.403151  | 3.470828 | 1           | 3.776681  | 6.765003 | -3.436089 |
| 7           | -1.574554 | -0.053387 | 3.295354 | 7           | 1.842902  | 5.208748 | -3.618109 |
| 6           | -1.054936 | -1.317645 | 3.220142 | 6           | 1.019261  | 4.120342 | -3.722976 |
| 6           | -3.097976 | 1.497085  | -0.309350 | 6           | 1.731854  | 7.899708 | 3.080344 |
| 1           | -3.153362 | 2.121525  | -1.214025 | 1           | 2.237432  | 8.214789 | 2.154849 |
| 1           | -3.237622 | 2.138749  | 0.573936 | 1           | 2.258830  | 8.340305 | 3.940343 |
| 1           | -3.890598 | 0.735784  | -0.339369 | 1           | 0.690353  | 8.251641 | 3.068085 |
| 7           | -1.812428 | 0.824310  | -0.242286 | 7           | 1.729559  | 6.450787 | 3.182286 |
| 6           | -1.558860 | -0.533163 | -0.217259 | 6           | 0.643040  | 5.601175 | 3.254976 |
| 1           | -2.374154 | -1.257747 | -0.248700 | 1           | -0.376382 | 5.990101 | 3.239851 |
| 7           | -0.264054 | -0.834513 | -0.153336 | 7           | 0.974387  | 4.315033 | 3.341418 |
| 6           | 0.350980  | 0.401445  | -0.136259 | 6           | 2.354694  | 4.338981 | 3.323193 |
| 6           | 1.757867  | 0.740471  | -0.073224 | 6           | 3.305706  | 3.248312 | 3.388467 |
| 8           | 2.758335  | 0.041394  | -0.019341 | 8           | 3.148301  | 2.039912 | 3.475302 |
| 7           | 1.889913  | 2.171910  | -0.080791 | 7           | 4.636076  | 3.790257 | 3.334426 |
| 1           | 2.859539  | 2.481690  | -0.038081 | 1           | 5.359018  | 3.073612 | 3.376141 |
| 6           | 0.878924  | 3.104494  | -0.137420 | 6           | 4.995682  | 5.115474 | 3.236956 |
| 7           | 1.253639  | 4.419403  | -0.132428 | 7           | 6.334903  | 5.388730 | 3.201697 |
| 1           | 2.218471  | 4.709824  | -0.089758 | 1           | 7.038459  | 4.667420 | 3.243972 |
| 1           | 0.519643  | 5.112632  | -0.173698 | 1           | 6.610308  | 6.358299 | 3.130238 |
| 7           | -0.402710 | 2.801058  | -0.194895 | 7           | 4.134131  | 6.111531 | 3.177260 |
| 6           | -0.587297 | 1.444622  | -0.190527 | 6           | 2.845980  | 5.650675 | 3.225095 |
Table 6: Coordinates (Angstrom) of G-quadruplex 2MB2. Second layer.

| Atomic num. | X      | Y      | Z      | Atomic num. | X      | Y      | Z      |
|-------------|--------|--------|--------|-------------|--------|--------|--------|
| 6           | 6.403772 | 7.893023 | -0.415215 | 6           | 12.125116 | 2.886545 | 3.266823 |
| 1           | 7.049051 | 7.916503 | -1.306557 | 1           | 12.527775 | 2.364080 | 2.385731 |
| 1           | 7.024049 | 8.069236 | 0.476768 | 1           | 12.505761 | 2.395505 | 4.175348 |
| 1           | 5.640577 | 8.680523 | -0.493360 | 1           | 12.451516 | 3.936300 | 3.252405 |
| 7           | 5.734173 | 6.608008 | -0.314547 | 7           | 10.673102 | 2.853114 | 3.249549 |
| 6           | 4.377395 | 6.349556 | -0.311433 | 6           | 9.794306 | 3.918243 | 3.220037 |
| 1           | 3.650859 | 7.159280 | -0.390115 | 1           | 10.158334 | 4.968641 | 3.206453 |
| 7           | 4.079223 | 5.056819 | -0.204897 | 7           | 8.513829 | 3.553320 | 3.210659 |
| 6           | 5.316615 | 4.448388 | -0.135441 | 6           | 8.572641 | 2.176164 | 3.235600 |
| 6           | 5.659057 | 3.046467 | -0.010572 | 6           | 7.936777 | 1.198647 | 3.239615 |
| 8           | 4.962462 | 2.045699 | 0.065373 | 8           | 6.288776 | 1.326194 | 3.222433 |
| 7           | 7.090739 | 2.920590 | 0.020281 | 7           | 8.080312 | -0.117822 | 3.269826 |
| 1           | 7.402871 | 1.954696 | 0.107381 | 1           | 7.380402 | -0.858139 | 3.274126 |
| 6           | 8.020803 | 3.928303 | -0.053371 | 6           | 9.417375 | -0.444607 | 3.292011 |
| 7           | 9.336555 | 3.564400 | -0.003372 | 7           | 9.724982 | -1.775646 | 3.319182 |
| 1           | 9.629314 | 2.603209 | 0.080353 | 1           | 9.019908 | -2.497602 | 3.323171 |
| 1           | 10.027954 | 4.299351 | -0.056624 | 1           | 10.703529 | -2.027934 | 3.335633 |
| 7           | 7.714254 | 5.209935 | -0.167048 | 7           | 10.393878 | 0.441154 | 3.28467 |
| 6           | 6.357444 | 5.388526 | -0.201366 | 6           | 8.994759 | 1.171419 | 3.259976 |
| 6           | 9.799810 | 5.400193 | -3.625789 | 6           | 12.203566 | -1.681881 | 0.115429 |
| 1           | 10.425291 | 5.101525 | -4.480774 | 1           | 12.277459 | -2.362728 | -0.746206 |
| 1           | 10.356925 | 5.211727 | -2.695450 | 1           | 12.294398 | -2.692998 | 1.041338 |
| 1           | 9.561856 | 6.470917 | -3.700994 | 1           | 13.015105 | -0.941606 | 0.069332 |
| 7           | 8.556826 | 4.684695 | -3.627000 | 7           | 10.933217 | -0.978803 | 0.009895 |
| 6           | 7.265767 | 5.132977 | -3.706332 | 6           | 10.712108 | 0.383589 | 0.022403 |
| 1           | 7.070956 | 6.204120 | -3.779910 | 1           | 11.545453 | 1.086640 | -0.021970 |
| 7           | 6.351455 | 4.181749 | -3.683252 | 7           | 9.423560 | 0.716816 | 0.017324 |
| 6           | 7.070775 | 3.017706 | -3.583230 | 6           | 8.778327 | -0.501796 | 0.086662 |
| 6           | 6.628718 | 1.639958 | -3.515114 | 6           | 7.362210 | -0.805120 | 0.115818 |
| 8           | 5.511512 | 1.145742 | -3.527389 | 8           | 6.377972 | -0.828156 | 0.087637 |
| 7           | 7.782425 | 0.787842 | -3.418337 | 7           | 7.195632 | -2.230971 | 0.191371 |
| 1           | 7.542766 | -0.201015 | -3.366476 | 1           | 6.217813 | -2.516025 | 0.215426 |
| 6           | 9.104503 | 1.170460 | -3.391328 | 6           | 8.184961 | -3.187332 | 0.231613 |
| 7           | 10.032517 | 0.171079 | -3.294103 | 7           | 7.778332 | -4.490777 | 0.303092 |
| 1           | 9.778816 | -0.803682 | -3.243650 | 1           | 6.805776 | -4.756619 | 0.326099 |
| 1           | 11.006166 | 0.440524 | -3.273451 | 1           | 8.496215 | -5.201241 | 0.333149 |
| 7           | 9.511822 | 2.422757 | -3.453030 | 7           | 9.474874 | -2.916411 | 0.205335 |
| 6           | 8.449485 | 3.281055 | -3.546690 | 6           | 9.692230 | -1.566756 | 0.133254 |
Table 7: Coordinates (Angstrom) of G-quadruplex 2MB2. Third layer.

| Atomic num. | X      | Y      | Z      | Atomic num. | X      | Y      | Z      |
|-------------|--------|--------|--------|-------------|--------|--------|--------|
| 6           | 10.264334 | -5.881469 | -2.84563 | 6           | 2.674049 | -7.963378 | -0.010491 |
| 1           | 10.039485 | -6.645291 | -3.604461 | 1           | 2.047804 | -8.037974 | -0.912533 |
| 1           | 10.001309 | -6.279392 | -1.852644 | 1           | 2.035104 | -8.090235 | 0.876687  |
| 1           | 11.336835 | -5.641151 | -2.871385 | 1           | 3.439105 | -8.752751 | -0.028118 |
| 7           | 9.511502  | -4.668916 | -3.114232 | 7           | 3.340750 | -6.673621 | 0.031913  |
| 6           | 9.996512  | -3.400940 | -3.368503 | 6           | 4.697034 | -6.413138 | 0.049148  |
| 1           | 11.069435 | -3.202881 | -3.386490 | 1           | 5.425480 | -7.225379 | 0.030594  |
| 7           | 9.043636  | -2.495722 | -3.578340 | 7           | 4.992262 | -5.115963 | 0.089132  |
| 6           | 7.877692  | -3.224188 | -3.451955 | 6           | 3.753385 | -4.506665 | 0.098136  |
| 6           | 6.497612  | -2.800442 | -3.570178 | 6           | 3.407703 | -3.100507 | 0.136754  |
| 8           | 6.002500  | -1.709366 | -3.073201 | 8           | 4.102054 | -2.095893 | 0.171026  |
| 7           | 5.644143  | -3.936350 | -3.351521 | 7           | 1.975629 | -2.975485 | 0.130241  |
| 1           | 4.653617  | -3.708249 | -3.420750 | 1           | 1.661260 | -2.006746 | 0.156306  |
| 6           | 6.027484  | -5.228869 | -3.073201 | 6           | 1.047819 | -3.991788 | 0.093971  |
| 7           | 5.026490  | -6.144683 | -2.903731 | 7           | -0.268874 | -3.623355 | 0.095836  |
| 1           | 4.050083  | -5.902732 | -2.975545 | 1           | -0.563859 | -2.659316 | 0.121451  |
| 1           | 5.296447  | -7.096645 | -2.699013 | 1           | -0.958636 | -4.361289 | 0.068937  |
| 7           | 7.281901  | -5.619432 | -2.964288 | 7           | 1.357319 | -5.272776 | 0.058752  |
| 6           | 8.141568  | -4.572987 | -3.164123 | 6           | 2.714638 | -5.405748 | 0.063188  |
| 6           | 7.189287  | -7.496018 | 3.367719  | 6           | -0.724050 | -5.752736 | -3.318720 |
| 1           | 6.674313  | -7.908501 | 2.486762  | 1           | -1.341779 | -5.485040 | -4.189453 |
| 1           | 6.713007  | -7.894807 | 4.276319  | 1           | -1.281003 | -5.511312 | -2.400647 |
| 1           | 8.247620  | -7.793068 | 3.347109  | 1           | -0.503448 | -6.829549 | -3.341921 |
| 7           | 7.115512  | -6.045422 | 3.358216  | 7           | 0.531091 | -5.022423 | -3.350711 |
| 6           | 8.155711  | -5.137253 | 3.328774  | 6           | 1.814283 | -5.530824 | -3.401724 |
| 1           | 9.193943  | -5.472507 | 3.308891  | 1           | 1.991736 | -6.607277 | -3.423455 |
| 7           | 7.757368  | -3.867315 | 3.327670  | 7           | 2.760302 | -4.594806 | -3.420214 |
| 6           | 6.380498  | -3.965253 | 3.358185  | 6           | 2.043545 | -3.415534 | -3.378661 |
| 6           | 5.37328   | -2.923146 | 3.371985  | 6           | 2.507918 | -2.043461 | -3.374412 |
| 8           | 5.467446  | -1.705099 | 3.360639  | 8           | 3.633114 | -1.568589 | -3.405728 |
| 7           | 4.073910  | -3.536257 | 3.404783  | 7           | 1.368037 | -1.169089 | -3.322943 |
| 1           | 3.314487  | -2.857202 | 3.416007  | 1           | 1.623714 | -0.182903 | -3.317245 |
| 6           | 3.784444  | -4.881974 | 3.421339  | 6           | 0.039780 | -1.528478 | -3.283056 |
| 7           | 2.461683  | -5.226578 | 3.452576  | 7           | -0.872026 | -0.510669 | -3.237231 |
| 1           | 1.721369  | -4.541825 | 3.463344  | 1           | -0.602536 | 0.461142  | -3.232213 |
| 1           | 2.237614  | -6.211798 | 3.464960  | 1           | -1.850025 | -0.762986 | -3.207684 |
| 7           | 4.696926  | -5.833386 | 3.408888  | 7           | -0.387823 | -2.775517 | -3.286718 |
| 6           | 5.958849  | -5.303689 | 3.377550  | 6           | 0.660590 | -3.654431 | -3.35158  |
| Atomic num. | X       | Y       | Z       | Atomic num. | X       | Y       | Z       |
|------------|---------|---------|---------|------------|---------|---------|---------|
| 6          | 11.972350 | -1.982580 | 4.206760 | 6          | 8.050410 | -6.764150 | -3.986640 |
| 1          | 12.110290 | -2.882020 | 3.587570 | 1          | 7.715160 | -6.940330 | -5.020800 |
| 1          | 11.883200 | -2.287380 | 5.260600 | 1          | 7.453850 | -7.392570 | -3.307950 |
| 1          | 12.840590 | -1.318550 | 4.088600 | 1          | 9.113150 | -7.030380 | -3.894760 |
| 7          | 10.780530 | -1.264630 | 3.789800 | 7          | 7.892910 | -5.362340 | -3.640410 |
| 6          | 10.684360 | 0.029460  | 3.314430 | 6          | 8.867420 | -4.463020 | -3.251430 |
| 1          | 11.570800 | 0.657440  | 3.213920 | 1          | 9.912530 | -4.766620 | -3.174800 |
| 7          | 9.441270  | 0.398520  | 3.016880 | 7          | 8.399850 | -3.242460 | -3.003900 |
| 6          | 8.694380  | -0.723880 | 3.314430 | 6          | 7.045470 | -3.363980 | -3.241910 |
| 6          | 7.268100  | -0.949990 | 3.201200 | 6          | 5.900240 | -2.376670 | -3.142170 |
| 8          | 6.360470  | -0.226120 | 2.802710 | 8          | 6.011760 | -1.196470 | -2.827160 |
| 7          | 6.975480  | -2.288220 | 3.637120 | 7          | 4.742070 | -2.995730 | -3.496200 |
| 1          | 5.983850  | -2.515690 | 3.583370 | 1          | 3.952310 | -2.353980 | -3.447230 |
| 6          | 7.867000  | -3.232510 | 4.093770 | 6          | 4.534650 | -4.303330 | -3.873250 |
| 7          | 7.348210  | -4.445070 | 4.454320 | 7          | 3.248150 | -4.663100 | -4.164630 |
| 1          | 6.363510  | -4.654640 | 4.395150 | 1          | 2.476930 | -4.015460 | -4.111280 |
| 1          | 7.993640  | -5.145840 | 4.791010 | 1          | 3.084300 | -5.620660 | -4.442570 |
| 7          | 9.165690  | -3.031610 | 4.198640 | 7          | 5.491490 | -5.205500 | -3.965500 |
| 6          | 9.501630  | -1.767430 | 3.794920 | 6          | 6.707100 | -4.667890 | -3.637960 |
| 6          | 10.250340 | -6.200190 | 1.457250 | 6          | -2.507820 | -3.932410 | -3.542700 |
| 1          | 10.646130 | -5.730080 | 2.370360 | 1          | -2.827990 | -3.703550 | -4.570580 |
| 1          | 11.005460 | -6.119500 | 0.660560 | 1          | -3.159380 | -3.391900 | -2.839320 |
| 1          | 10.035240 | -7.260350 | 1.653500 | 1          | -2.591630 | -5.013970 | -3.364040 |
| 7          | 9.019280  | -5.545970 | 1.049530 | 7          | -1.123610 | -3.537240 | -3.348870 |
| 6          | 7.762010  | -6.100890 | 0.911700 | 6          | -0.049090 | -4.331880 | -3.000140 |
| 1          | 7.589200  | -7.158710 | 1.116310 | 1          | -0.173580 | -5.402710 | -2.831210 |
| 7          | 6.833740  | -5.231840 | 0.518690 | 7          | 1.098850 | -3.665790 | -2.900310 |
| 6          | 7.535070  | -4.048880 | 0.396650 | 6          | 0.741650 | -2.366860 | -3.202510 |
| 6          | 7.078450  | -2.732410 | 0.000860 | 6          | 1.552830 | -1.168290 | -3.262950 |
| 8          | 5.975030  | -2.321270 | -0.324670 | 8          | 2.744920 | -0.958750 | -3.067660 |
| 7          | 8.194860  | -1.827240 | 0.029310 | 7          | 0.713060 | -0.058630 | -3.623490 |
| 1          | 7.943210  | -0.877420 | -0.239900 | 1          | 1.222310 | 0.821650  | -3.684470 |
| 6          | 9.497210  | -2.116410 | 0.368870 | 6          | -0.639560 | -0.081930 | -3.878210 |
| 7          | 10.389900 | -1.081890 | 0.320850 | 7          | -1.224900 | 1.109770  | -4.204780 |
| 1          | 10.124730 | -0.146720 | 0.052140 | 1          | -0.706490 | 1.973010  | -4.269040 |
| 1          | 11.348810 | -1.282810 | 0.568130 | 1          | -2.217500 | 1.104370  | -4.393810 |
| 7          | 9.917650  | -3.312650 | 0.729680 | 7          | -1.382070 | -1.169940 | -3.824490 |
| 6          | 8.890910  | -4.218030 | 0.720110 | 6          | -0.629960 | -2.261900 | -3.483950 |
Table 9: Coordinates (Angstrom) of G-quadruplex 143D. Second layer

| Atomic num. | X       | Y       | Z       | Atomic num. | X       | Y       | Z       |
|------------|---------|---------|---------|------------|---------|---------|---------|
| 6          | -1.232110 | -5.128430 | 0.776320 | 6          | 6.023280  | 7.614230 | 3.168110 |
| 1          | -0.947920  | -5.516940 | 1.766130 | 1          | 6.787090  | 7.724880 | 2.383400 |
| 1          | -1.027060  | -5.900890 | 0.019560 | 1          | 6.526550  | 7.516710 | 4.142090 |
| 1          | -2.304160  | -4.884660 | 0.771310 | 1          | 5.374530  | 8.501800 | 3.177060 |
| 7          | -0.481660  | -3.921380 | 0.476970 | 7          | 5.203000  | 6.444060 | 2.908080 |
| 6          | -0.968190  | -2.654430 | 0.220500 | 6          | 3.838940  | 6.386210 | 2.699150 |
| 1          | -2.040590  | -2.452820 | 0.224770 | 1          | 3.229060  | 7.290910 | 2.715890 |
| 7          | -0.017380  | -1.754770 | -0.020360 | 7          | 3.382110  | 5.154480 | 2.485680 |
| 6          | 1.148760   | -2.485950 | 0.087540 | 6          | 4.518870  | 4.374660 | 2.561790 |
| 6          | 2.527160   | -2.068280 | -0.066740 | 6          | 4.676710  | 2.942190 | 2.415610 |
| 8          | 3.020280   | -0.981480 | -0.328000 | 8          | 3.866070  | 2.056300 | 2.190660 |
| 7          | 3.381680   | -3.204820 | 0.144390 | 7          | 6.065420  | 2.610090 | 2.582040 |
| 1          | 4.371110   | -2.980910 | 0.050330 | 1          | 6.248930  | 1.612080 | 2.491100 |
| 6          | 3.000550   | -4.493030 | 0.444850 | 6          | 7.106590  | 3.473360 | 2.838470 |
| 7          | 4.002160   | -5.410520 | 0.601160 | 7          | 8.350740  | 2.918890 | 2.957150 |
| 1          | 4.977460   | -5.172740 | 0.504690 | 1          | 8.515840  | 1.928330 | 2.864360 |
| 1          | 3.733820   | -6.359360 | 0.821900 | 1          | 9.122510  | 3.543350 | 3.145400 |
| 7          | 1.747670   | -4.878060 | 0.586260 | 7          | 6.968110  | 4.777530 | 2.972320 |
| 6          | 0.887100   | -3.830760 | 0.395030 | 6          | 5.659560  | 5.150750 | 2.822640 |
| 6          | 2.236320   | -7.612410 | 5.801350 | 6          | 10.993390 | 5.273920 | -0.63590 |
| 1          | 1.703930   | -8.005770 | 4.921990 | 1          | 10.621550 | 5.896970 | 0.191040 |
| 1          | 1.498860   | -7.353610 | 6.576330 | 1          | 10.780040 | 5.783860 | -1.58837 |
| 1          | 2.922550   | -8.379090 | 6.188650 | 1          | 12.078520 | 5.132230 | -0.530940 |
| 7          | 3.011520   | -6.439900 | 5.435220 | 7          | 10.351900 | 3.971010 | -0.610910 |
| 6          | 4.376780   | -6.254200 | 5.531260 | 6          | 10.943490 | 2.729900 | -0.479330 |
| 1          | 5.024740   | -7.040640 | 5.921610 | 1          | 12.025360 | 2.631160 | -0.376690 |
| 7          | 4.785110   | -5.059250 | 5.110810 | 7          | 10.076750 | 1.719940 | -0.492330 |
| 6          | 3.613940   | -4.440330 | 4.721640 | 6          | 8.856430  | 2.348340 | -0.640960 |
| 6          | 3.397910   | -3.117140 | 4.173240 | 6          | 7.523890  | 1.786460 | -0.732930 |
| 8          | 4.174920   | -2.211870 | 3.912410 | 8          | 7.127550  | 0.631470 | -0.685820 |
| 7          | 1.992190   | -2.940870 | 3.929490 | 7          | 6.578180  | 2.858340 | -0.876300 |
| 1          | 1.767950   | -2.026100 | 3.541080 | 1          | 5.615160  | 2.532260 | -0.941340 |
| 6          | 0.983150   | -3.847950 | 4.161990 | 6          | 6.846080  | 4.207200 | -0.938170 |
| 7          | -0.286600  | -3.449960 | 3.847700 | 7          | 5.773130  | 5.041530 | -1.08677 |
| 1          | -0.492080  | -2.540370 | 3.463650 | 1          | 4.825330  | 4.702740 | -1.149660 |
| 1          | -1.035170  | -4.107910 | 4.014280 | 1          | 5.958160  | 6.033810 | -1.133370 |
| 7          | 1.174600   | -5.053130 | 4.660830 | 7          | 8.056820  | 4.723390 | -0.863150 |
| 6          | 2.501600   | -5.275560 | 4.913010 | 6          | 9.009090  | 3.742940 | -0.716740 |
### Table 10: Coordinates (Angstrom) of Gquadruplex 143D. Third layer.

| Atomic num. | X   | Y         | Z         | Atomic num. | X   | Y         | Z         |
|-------------|-----|-----------|-----------|-------------|-----|-----------|-----------|
| 6           | 11.967630 | 3.831900 | -4.250140 | 6           | -0.391950 | 6.167290 | -0.418760 |
| 1           | 12.424150 | 3.196200 | -5.024020 | 1           | -0.762450 | 6.005690 | 0.604980  |
| 1           | 12.378670 | 3.547780 | -3.269450 | 1           | -1.157520 | 5.824770 | -1.131510 |
| 1           | 12.202270 | 4.886220 | -4.453520 | 1           | -0.197980 | 7.238200 | -0.574470 |
| 7           | 10.524230 | 3.669610 | -4.255040 | 7           | 0.847110  | 5.437840 | -0.624670 |
| 6           | 9.557110  | 4.631330 | -4.472820 | 6           | 2.089060  | 5.940820 | -0.959630 |
| 1           | 9.831060  | 5.668340 | -4.673520 | 1           | 2.240940  | 7.011470 | -1.105740 |
| 1           | 8.312970  | 4.162580 | -4.411140 | 7           | 3.030580  | 5.007380 | -1.076590 |
| 6           | 8.490410  | 2.820970 | -4.137710 | 6           | 2.354540  | 3.856360 | -0.800700 |
| 6           | 7.509910  | 1.770910 | -3.952710 | 6           | 2.834720  | 2.469410 | -0.767600 |
| 8           | 6.288820  | 1.786990 | -3.987590 | 8           | 3.941950  | 1.994400 | -0.970020 |
| 7           | 8.197730  | 0.536760 | -3.687580 | 7           | 1.739820  | 1.601970 | -0.428120 |
| 1           | 7.564380  | -0.248710 | -3.546610 | 1           | 2.008760  | 0.620160 | -0.387010 |
| 6           | 9.557670  | 0.337010 | -3.612300 | 6           | 0.436750  | 1.962520 | -0.169220 |
| 7           | 9.978850  | -0.936270 | -3.346240 | 7           | -0.432790 | 0.951860 | 0.133920  |
| 1           | 9.338700  | -1.703400 | -3.209120 | 1           | -1.506500 | -0.015670 | 0.170530  |
| 1           | 10.975200 | -1.094400 | -3.288730 | 1           | -1.392000 | 1.205100 | 0.325770  |
| 7           | 10.453890 | 1.289200 | -3.779870 | 7           | -0.005090 | 3.204260 | -0.198060 |
| 6           | 9.851540  | 2.491440 | -4.036390 | 6           | 1.000480  | 4.076420 | -0.517720 |
| 6           | 0.642570  | 7.050140 | -4.597350 | 6           | -3.802880 | 1.798490 | 3.877630  |
| 1           | 1.011050  | 7.309980 | -5.601400 | 1           | -3.999530 | 2.359630 | 2.951420  |
| 1           | 1.165650  | 7.672330 | -3.855260 | 1           | -3.671620 | 2.513030 | 4.704460  |
| 1           | -0.438440 | 7.242580 | -4.541570 | 1           | -4.654430 | 1.137850 | 4.094730  |
| 7           | 0.876640  | 5.642540 | -4.325970 | 7           | -2.610910 | 0.982400 | 3.726090  |
| 6           | -0.052640 | 4.661520 | -4.040120 | 6           | -2.497260 | -0.390530 | 3.824960  |
| 1           | -1.117980 | 4.893070 | -3.993850 | 1           | -3.367370 | -1.012200 | 4.041220  |
| 7           | 0.482790  | 3.459880 | -3.838170 | 7           | -1.259390 | -0.840160 | 3.632760  |
| 6           | 1.835480  | 3.681100 | -4.003840 | 6           | -0.534640 | 0.310950 | 3.396470  |
| 6           | 2.948050  | 2.758180 | -3.910830 | 6           | 0.876470  | 0.481890 | 3.117560  |
| 8           | 2.990450  | 1.561980 | -3.663550 | 8           | 1.786710  | -0.326880 | 3.018070  |
| 7           | 4.167170  | 3.475350 | -4.167590 | 7           | 1.147710  | 1.882930 | 2.944230  |
| 1           | 4.994590  | 2.882990 | -4.117920 | 1           | 2.127790  | 2.076070 | 2.744000  |
| 6           | 4.304450  | 4.814040 | -4.457540 | 6           | 0.250320  | 2.924000 | 3.020990  |
| 7           | 5.576100  | 5.271510 | -4.665060 | 7           | 0.747600  | 4.181340 | 2.817950  |
| 1           | 6.385220  | 4.671840 | -4.612260 | 1           | 1.721080  | 4.355890 | 2.620580  |
| 1           | 5.688630  | 6.252700 | -4.878640 | 1           | 0.097690  | 4.953170 | 2.871980  |
| 7           | 3.295240  | 5.657900 | -4.543300 | 7           | -1.034620 | 2.773620 | 3.274500  |
| 6           | 2.104380  | 5.025550 | -4.306640 | 6           | -1.349860 | 1.452950 | 3.449030  |
Optimized Guanine

The geometrical structure have been optimized using the B3LYP exchange-correlation (xc) functional and the cc-pVTZ basis set. TD-DFT simulations have been done using the CAM-B3LYP xc-functional and the aug-cc-pVTZ basis set. The cubic grid, centered on the molecular structure, have a spacing of 0.1 a.u., a side of 40 a.u., and 68921 grid points. The annular shaped electron beam have the following dimensions: 7 a.u. of radius and 3 a.u. thick.

Table 11: Excitation energy (eV), oscillator strength and OAM resolved transition rates of the optimized guanine structure.

| Transition | Guanine energy | Osc. Str. | Orbital angular momentum |
|------------|----------------|-----------|--------------------------|
| $S_1 \rightarrow S_0$ | 5.056 | 0.133 | 0.0 | 0.7 | 16.0 | 0.0 | 16.0 | 0.7 | 0.0 |
| $S_2 \rightarrow S_0$ | 5.167 | 0.023 | 0.0 | 0.2 | 2.5 | 0.0 | 2.5 | 0.2 | 0.0 |
| $S_3 \rightarrow S_0$ | 5.514 | 0.079 | 0.1 | 0.5 | 8.4 | 0.0 | 8.4 | 0.5 | 0.1 |
| $S_4 \rightarrow S_0$ | 5.553 | 0.000 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| $S_5 \rightarrow S_0$ | 5.557 | 0.244 | 0.2 | 1.2 | 26.7 | 0.0 | 26.7 | 1.2 | 0.2 |

Guanine tetramer

The geometry of the flat guanine tetramer has been obtained optimizing a monolayer of guanine on top of a gold slab with four layers of Au(111), as detailed in ref. 3. TD-DFT simulations have been done using the CAM-B3LYP xc-functional and the 6-311G(d) basis set. The cubic grid, centered on the molecular structure, have a spacing of 0.1 a.u., a side of 50 a.u. and 132651 grid points. The annular shaped electron beam have the following dimensions: 20 a.u. of radius and 3 a.u. thick. In the case of the monomer extracted from the structure of the tetramer, we used the same computational protocol of the total system including the grid cube: therefore this last was centered on the total structure.
Table 12: Excitation energy (eV), oscillator strength and OAM resolved transition rates of the guanine monomer extracted from the tetramer.

| Guanine Monomer | Orbital angular momentum |
|-----------------|--------------------------|
| Transition      | energy | Osc. Str. | -3 | -2 | -1 | 0  | 1  | 2  | 3  |
| S₁ ← S₀        | 5.057  | 0.163     | 0.0 | 0.6| 19.9| 0.0| 19.9| 0.6| 0.0 |
| S₂ ← S₀        | 5.358  | 0.001     | 0.0 | 0.0| 0.1 | 0.0| 0.1 | 0.0| 0.0 |
| S₃ ← S₀        | 5.507  | 0.290     | 0.2 | 1.5| 32.5| 0.0| 32.5| 1.5| 0.2 |
| S₄ ← S₀        | 5.710  | 0.008     | 0.1 | 0.8| 0.0 | 0.0| 0.8 | 0.0| 0.0 |
| S₅ ← S₀        | 6.233  | 0.002     | 0.0 | 0.0| 0.0 | 0.0| 0.0 | 0.0| 0.0 |

Table 13: Excitation energy (eV), oscillator strength and OAM resolved transition rates of the guanine tetramer structure.

| Guanine tetramer | Orbital angular momentum |
|-----------------|--------------------------|
| Transition      | energy | Osc. Str. | -4 | -3 | -2 | -1 | 0  | 1  | 2  | 3  | 4  |
| S₁ ← S₀        | 5.061  | 0.002     | 0.0 | 0.0| 4.7 | 0.1| 0.1 | 4.7| 0.0| 0.0 |
| S₂ ← S₀        | 5.074  | 0.271     | 0.0 | 0.2| 0.0 | 12.1| 0.0| 12.1| 0.0| 0.2| 0.0 |
| S₃ ← S₀        | 5.086  | 0.306     | 0.0 | 0.2| 0.0 | 13.6| 0.0| 13.6| 0.0| 0.2| 0.0 |
| S₄ ← S₀        | 5.097  | 0.002     | 0.0 | 0.0| 0.1 | 0.1| 0.1 | 0.1| 0.0| 0.0 |
| S₅ ← S₀        | 5.357  | 0.000     | 1.5 | 0.0| 0.3 | 0.0| 0.4 | 0.0| 0.3 | 0.0| 1.5 |
| S₆ ← S₀        | 5.378  | 0.721     | 0.0 | 2.8| 0.0 | 30.3| 0.0| 30.3| 0.0| 2.8| 0.0 |
| S₇ ← S₀        | 5.394  | 0.721     | 0.0 | 3.6| 0.0 | 30.2| 0.0| 30.2| 0.0| 3.6| 0.0 |
| S₈ ← S₀        | 5.417  | 0.000     | 0.1 | 0.0| 22.3| 0.0| 0.0 | 0.0| 22.3| 0.0| 0.1 |

**Alanine enantiomers**

The geometrical structure have been optimized using the B3LYP exchange-correlation (xc) functional and the cc-pVTZ basis set. TD-DFT simulations have been done using the CAM-B3LYP xc-functional and the cc-pVTZ basis set. The cubic grid, centered on the molecular structure, have a spacing of 0.1 a.u., a side of 80 a.u. and 531441 grid points. The annular shaped electron beam have the following dimensions: 7 a.u. of radius and 3 a.u. thick.

**G-quadruplex structures**

The geometries of the guanine core of parallel and anti-parallel G-quadruplexes have been extracted from the NMR structures of PDB files: PDB ID 2MB2 and 143D, respectively. Therefore, they have been refined by projecting the MP2/cc-pVDZ optimized geometry of
Table 14: Excitation energy (eV), oscillator strength and OAM resolved transition rates of the L-alanine.

| L-alanine | Orbital angular momentum |
|-----------|-------------------------|
| Transition energy | Osc. Str. | -3 | -2 | -1 | 0 | 1 | 2 | 3 |
| \( S_1 \leftarrow S_0 \) | 5.7623 | 0.0013 | 0.02 | 0.31 | 1.71 | 0.96 | 1.70 | 0.31 | 0.02 |
| \( S_2 \leftarrow S_0 \) | 7.0424 | 0.0154 | 0.89 | 3.23 | 30.59 | 3.55 | 29.89 | 3.18 | 0.88 |
| \( S_3 \leftarrow S_0 \) | 7.9932 | 0.0227 | 1.54 | 1.26 | 33.99 | 9.68 | 33.79 | 1.28 | 1.53 |
| \( S_4 \leftarrow S_0 \) | 8.0665 | 0.0032 | 0.15 | 0.73 | 4.33 | 0.39 | 4.14 | 0.74 | 0.15 |
| \( S_5 \leftarrow S_0 \) | 8.4068 | 0.0087 | 0.68 | 2.05 | 10.09 | 0.6 | 10.4 | 2.08 | 0.69 |

Table 15: Excitation energy (eV), oscillator strength and OAM resolved transition rates of the D-alanine.

| D-alanine | Orbital angular momentum |
|-----------|-------------------------|
| Transition energy | Osc. Str. | -3 | -2 | -1 | 0 | 1 | 2 | 3 |
| \( S_1 \leftarrow S_0 \) | 5.7623 | 0.0013 | 0.02 | 0.33 | 1.64 | 1.08 | 1.65 | 0.33 | 0.02 |
| \( S_2 \leftarrow S_0 \) | 7.0424 | 0.0154 | 0.76 | 3.25 | 30.01 | 3.33 | 30.7 | 3.3 | 0.77 |
| \( S_3 \leftarrow S_0 \) | 7.9932 | 0.0227 | 1.61 | 1.57 | 34.2 | 8.5 | 34.37 | 1.55 | 1.61 |
| \( S_4 \leftarrow S_0 \) | 8.0665 | 0.032 | 0.17 | 0.7 | 4.15 | 0.35 | 4.34 | 0.69 | 0.17 |
| \( S_5 \leftarrow S_0 \) | 8.4068 | 0.0087 | 0.64 | 2.08 | 10.58 | 0.64 | 10.25 | 2.04 | 0.64 |

the guanine base to the NMR structure, as detailed in ref. 6.

All the TD-DFT calculations have been done employing the CAM-B3LYP xc-functional and the 6-31G(d) basis set. The cubic grid, centered on each supramolecular structure, have a spacing of 0.1 a.u., a side of 85 a.u. and 753571 grid points for both the structures. The annular shaped electron beam have the following dimensions: 24 a.u. of radius and 3 a.u. thick.
Table 16: Excitation energy (eV), oscillator strength and dichroic figure of merit (eq. (13) of main text) of the 2MB2 G-quadruplex.

| Transition | Energy | Osc. Str. | $|l| = 1$ | $|l| = 2$ | $|l| = 3$ |
|------------|--------|-----------|---------|---------|---------|
| $S_1 \leftarrow S_0$ | 4.938 | 0.004 | 5.9 | 0.7 | 2.2 |
| $S_2 \leftarrow S_0$ | 5.064 | 0.0208 | 0.8 | 1.3 | 2.8 |
| $S_3 \leftarrow S_0$ | 5.065 | 0.0001 | -0.9 | -0.3 | -2.3 |
| $S_4 \leftarrow S_0$ | 5.090 | 0.0007 | 2.2 | -0.4 | 2.2 |
| $S_5 \leftarrow S_0$ | 5.107 | 0.618 | 1.8 | 4.9 | 1.5 |
| $S_6 \leftarrow S_0$ | 5.137 | 0.0305 | 2.0 | -0.7 | 5.2 |
| $S_7 \leftarrow S_0$ | 5.143 | 0.0152 | 0.1 | 2.8 | 1.7 |
| $S_8 \leftarrow S_0$ | 5.151 | 0.0356 | 3.1 | 2.4 | 2.8 |
| $S_9 \leftarrow S_0$ | 5.153 | 0.0187 | 1.7 | -2.1 | 3.7 |
| $S_{10} \leftarrow S_0$ | 5.166 | 0.0338 | 2.6 | 4.2 | -7.2 |
| $S_{11} \leftarrow S_0$ | 5.174 | 0.0946 | 0.5 | -3.9 | -0.8 |
| $S_{12} \leftarrow S_0$ | 5.175 | 0.0241 | 1.8 | -0.2 | 0.7 |
| $S_{13} \leftarrow S_0$ | 5.181 | 0.0328 | -0.1 | -0.4 | -0.2 |
| $S_{14} \leftarrow S_0$ | 5.195 | 0.0909 | 0.8 | -2.6 | -0.6 |
| $S_{15} \leftarrow S_0$ | 5.207 | 0.0162 | -1.2 | 9.1 | -0.7 |

Table 17: Excitation energy (eV), oscillator strength and dichroic figure of merit (eq. (13) of main text) of the 143D G-quadruplex.

| Transition | Energy | Osc. Str. | $|l| = 1$ | $|l| = 2$ | $|l| = 3$ |
|------------|--------|-----------|---------|---------|---------|
| $S_1 \leftarrow S_0$ | 4.9987 | 0.1197 | 1.5 | 1.3 | 2.1 |
| $S_2 \leftarrow S_0$ | 5.0264 | 0.0315 | 3.0 | 7.9 | -2.9 |
| $S_3 \leftarrow S_0$ | 5.0938 | 0.0386 | 0.8 | 0.9 | 3.4 |
| $S_4 \leftarrow S_0$ | 5.1059 | 0.0386 | -1.1 | 1.0 | -1.0 |
| $S_5 \leftarrow S_0$ | 5.1232 | 0.0438 | 0.4 | -1.8 | -2.8 |
| $S_6 \leftarrow S_0$ | 5.1259 | 0.0390 | 0.7 | -0.2 | 0.5 |
| $S_7 \leftarrow S_0$ | 5.143 | 0.0400 | -0.8 | -0.6 | -2.3 |
| $S_8 \leftarrow S_0$ | 5.1715 | 0.0182 | 7.7 | -2.4 | 1.4 |
| $S_9 \leftarrow S_0$ | 5.1839 | 0.0444 | -0.7 | -4.1 | 2.5 |
| $S_{10} \leftarrow S_0$ | 5.1922 | 0.0155 | 7.4 | 2.9 | -1.8 |
| $S_{11} \leftarrow S_0$ | 5.1988 | 0.0118 | -4.4 | -4.6 | -1.2 |
| $S_{12} \leftarrow S_0$ | 5.2147 | 0.0544 | 0.4 | 0.0 | -1.2 |
| $S_{13} \leftarrow S_0$ | 5.2287 | 0.0308 | -1.1 | 0.5 | -1.9 |
| $S_{14} \leftarrow S_0$ | 5.2333 | 0.2754 | -1.0 | 0.1 | -2.0 |
| $S_{15} \leftarrow S_0$ | 5.2459 | 0.1652 | 0.2 | -2.7 | -2.1 |
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