# DMRG calculations of $\pi$-conjugated oligomers within the Pariser-Parr-Pople model

## Abstract

## 1 Introduction

## 2 Theory

## 3 Results and discussion

In this section we present the results of PPP-DMRG calculations for various $\pi$-conjugated oligomers. The DMRG-SCF calculations were done using the CHEMPS2 code developed by Wouters *et al.*[18] These are compared with the FCI, QCI and MRSDCI energies wherever applicable.

### 3.1 Trans-polyacetylene (t-PA)

| Polyene | State | QCI | FCI | DMRG |
|---|---|---|---|---|
| t-PA3 | $^1A_g1$ | -12.458343 | -12.458780 | -12.458780 |
| | $^3B_u1$ | -10.277544 | -10.277544 | -10.277544 |
| | $^1B_u1$ | -7.442250 | -7.442250 | -7.442250 |
| t-PA4 | $^1A_g1$ | -16.870505 | -16.872655 | -16.872655 |
| | $^3B_u1$ | -14.961765 | -14.963297 | -14.963297 |
| | $^1B_u1$ | -12.344219 | -12.344720 | -12.344720 |
| t-PA5 | $^1A_g1$ | -21.282937 | -21.288916 | -21.288916 |
| | $^3B_u1$ | -19.535982 | -19.545397 | -19.545397 |
| | $^1B_u1$ | -17.087380 | - | -17.096594 |
| t-PA6 | $^1A_g1$ | -25.693448 | -25.706021 | -25.706021 |
| | $^3B_u1$ | -24.044655 | -24.070730 | -24.070730 |
| | $^1B_u1$ | -21.833261 | - | -21.893976 |
| t-PA7 | $^1A_g1$ | -30.101084 | | -30.33384 |
| | $^3B_u1$ | -28.507653 | - | -28.560342 |
| | $^1B_u1$ | -26.480342 | | -26.593011 |
| t-PA8 | $^1A_g1$ | -34.505365 | | -34.538917 |
| | $^3B_u1$ | -32.936230 | - | -33.015621 |
| | $^1B_u1$ | -31.039913 | | -31.205700 |
| t-PA9 | $^1A_g1$ | -38.906042 | | -38.949195 |
| | $^3B_u1$ | -37.337582 | - | -37.435080 |
| | $^1B_u1$ | -35.531428 | | -35.732269 |

Table 1: Calculated energies of t-PA singlet and triplet states using standard parameters

## 3.2 Polyacenes

| Acene | State | QCI | FCI | DMRG |
|---|---|---|---|---|
| $Acene-2\ (scr)$ | $^1A_g1$ | -21.231665 | -21.245326 | -21.245326 |
| | $^1A_g2$ | -16.778122 | -16.879752 | -16.879752 |
| | $^1A_g3$ | -16.132909 | -16.230828 | -16.230828 |
| | $^1B_{3u}1$ | -17.973619 | -18.027494 | -18.027494 |
| | $^1B_{3u}2$ | -15.914066 | -15.945570 | -15.945570 |
| | $^1B_{3u}3$ | -15.494116 | -15.578208 | -15.578207 |
| | $^1B_{2u}1$ | -16.725197 | -16.731789 | -16.733495 |
| | $^1B_{2u}2$ | -15.098515 | -15.126994 | -15.131767 |
| | $^1B_{2u}3$ | -14.552948 | -14.685479 | -14.689363 |
| | $^1B_{1g}1$ | -16.399262 | -16.468476 | -16.468475 |
| | $^1B_{1g}2$ | -15.383603 | -15.496246 | -15.496246 |
| | $^1B_{1g}3$ | -14.852170 | -14.879300 | -14.879300 |
| | $^3B_{3u}1$ | -17.876041 | -17.917925 | -17.917925 |
| | $^3B_{3u}2$ | -16.442217 | -16.462533 | -16.462533 |
| | $^3B_{3u}3$ | -15.952453 | -16.037961 | -16.037961 |
| | $^3B_{2u}1$ | -19.118211 | -19.132710 | -19.140764 |
| | $^3B_{2u}2$ | -17.429214 | -17.477969 | -17.491411 |
| | $^3B_{2u}3$ | -15.625677 | -15.689570 | -15.696835 |
| | $^3B_{1g}1$ | -17.926667 | -17.969360 | -17.969360 |
| | $^3B_{1g}2$ | -16.366059 | -16.454480 | -16.454480 |
| | $^3B_{1g}3$ | -15.608042 | -15.631783 | -15.631782 |

Table 2: Acene 2 screened

| Acene | State | QCI | FCI | DMRG |
|---|---|---|---|---|
| $Acene-2\ (std)$ | $^1A_g1$ | -24.091644 | -24.095718 | -24.095718 |
| | $^1A_g2$ | -19.169754 | -19.203886 | -19.203886 |
| | $^1A_g3$ | -18.396669 | -18.425356 | -18.425356 |
| | $^1B_{3u}1$ | -20.471611 | -20.484839 | -20.484839 |
| | $^1B_{3u}2$ | -18.100980 | -18.110086 | -18.110086 |
| | $^1B_{3u}3$ | -17.785872 | -17.811819 | -17.811819 |
| | $^1B_{2u}1$ | -19.644644 | -19.647236 | -19.647470 |
| | $^1B_{2u}2$ | -17.989607 | -17.995415 | -17.996438 |
| | $^1B_{2u}3$ | -16.627363 | -16.670660 | -16.671862 |
| | $^1B_{1g}1$ | -18.724095 | -18.747290 | -18.747290 |
| | $^1B_{1g}2$ | -18.271346 | -18.277974 | -18.277974 |
| | $^1B_{1g}3$ | -17.479520 | -17.523428 | -17.523428 |
| | $^3B_{3u}1$ | -20.356551 | -20.366031 | -20.366031 |
| | $^3B_{3u}2$ | -19.331451 | -19.335137 | -19.335137 |
| | $^3B_{3u}3$ | -18.165555 | -18.187670 | -18.187670 |
| | $^3B_{2u}1$ | -21.561073 | -21.565198 | -21.567095 |
| | $^3B_{2u}2$ | -19.791947 | -19.804155 | -19.807521 |
| | $^3B_{2u}3$ | -17.820521 | -17.836750 | -17.838865 |
| | $^3B_{1g}1$ | -20.344651 | -20.356674 | -20.356674 |
| | $^3B_{1g}2$ | -18.627926 | -18.655666 | -18.655666 |
| | $^3B_{1g}3$ | -17.962789 | -17.969055 | -17.969055 |

Table 3: Acene 2 standard

| Acene | State | QCI | FCI | DMRG |
|---|---|---|---|---|
| $Acene-3\ (scr)$ | $^1A_g1$ | -30.017779 | -30.061883 | -30.065992 |
| | $^1A_g2$ | -26.344622 | -26.580694 | -26.596829 |
| | $^1A_g3$ | -25.562375 | -25.785483 | -25.808448 |
| | $^1B_{3u}1$ | -26.995622 | -27.152327 | -27.180474 |
| | $^1B_{3u}2$ | -25.398134 | -25.672074 | -25.697101 |
| | $^1B_{3u}3$ | -25.301162 | -25.415665 | -25.431778 |
| | $^1B_{2u}1$ | -26.486676 | -26.509510 | -26.529015 |
| | $^1B_{2u}2$ | -25.408516 | -25.559938 | -25.587811 |
| | $^1B_{2u}3$ | -24.130369 | -24.375672 | -24.403091 |
| | $^1B_{1g}1$ | -26.045376 | -26.196057 | -26.217492 |
| | $^1B_{1g}2$ | -25.158381 | -25.251164 | -25.265467 |
| | $^1B_{1g}3$ | -24.201908 | -24.543041 | -24.573129 |
| | $^3B_{3u}1$ | -26.877354 | -27.015887 | -27.036801 |
| | $^3B_{3u}2$ | -25.668673 | -25.782338 | -25.807015 |
| | $^3B_{3u}3$ | -25.541910 | -25.756962 | -25.771278 |
| | $^3B_{2u}1$ | -28.542994 | -28.581635 | -28.624790 |
| | $^3B_{2u}2$ | -26.648252 | -26.781800 | -26.821836 |
| | $^3B_{2u}3$ | -26.014098 | -26.182787 | -26.244931 |
| | $^3B_{1g}1$ | -27.360119 | -27.480001 | -27.505489 |
| | $^3B_{1g}2$ | -25.461580 | -25.714068 | -25.744532 |
| | $^3B_{1g}3$ | -25.409716 | -25.496690 | -25.510171 |

Table 4: Acene 3 screened

| Acene | State | QCI | FCI | DMRG |
|---|---|---|---|---|
| $Acene-3\ (std)$ | $^1A_g1$ | -33.969952 | -33.985884 | -33.987035 |
| | $^1A_g2$ | -29.990165 | -30.097752 | -30.103397 |
| | $^1A_g3$ | -28.910107 | -29.011066 | -29.019790 |
| | $^1B_{3u}1$ | -30.683392 | -30.737773 | -30.746781 |
| | $^1B_{3u}2$ | -28.978510 | -29.087312 | -29.095699 |
| | $^1B_{3u}3$ | -28.600876 | -28.642372 | -28.646600 |
| | $^1B_{2u}1$ | -30.314013 | -30.326309 | -30.330848 |
| | $^1B_{2u}2$ | -28.953764 | -29.009430 | -29.018437 |
| | $^1B_{2u}3$ | -28.249695 | -28.280688 | -28.288341 |
| | $^1B_{1g}1$ | -29.609817 | -29.672212 | -26.217492 |
| | $^1B_{1g}2$ | -29.151648 | -29.184569 | -25.265467 |
| | $^1B_{1g}3$ | -27.651668 | -27.717532 | -24.573129 |
| | $^3B_{3u}1$ | -30.533062 | -30.578404 | -30.585333 |
| | $^3B_{3u}2$ | -29.632707 | -29.658581 | -29.662281 |
| | $^3B_{3u}3$ | -29.024300 | -29.108608 | -29.118672 |
| | $^3B_{2u}1$ | -32.240745 | -32.256256 | -32.269389 |
| | $^3B_{2u}2$ | -30.273973 | -30.318924 | -30.332083 |
| | $^3B_{2u}3$ | -29.505684 | -29.563884 | -29.584404 |
| | $^3B_{1g}1$ | -30.988637 | -31.034231 | -31.042454 |
| | $^3B_{1g}2$ | -28.951647 | -29.055489 | -29.066312 |
| | $^3B_{1g}3$ | -28.919489 | -28.952258 | -28.955530 |

Table 5: Acene 3 standard

| State | QCI | FCI | DMRG |
|---|---|---|---|
| $^1A_g1$ | -38.748161 | - | -38.767953 |
| $^1A_g2$ | -35.639580 | - | -35.885093 |
| $^1A_g3$ | -34.826591 | - | -34.993326 |
| $^1B_{3u}1$ | -35.772049 | - | -35.969713 |
| $^1B_{3u}2$ | -34.774138 | - | -35.059273 |
| $^1B_{3u}3$ | -34.305058 | - | -34.494806 |
| $^1B_{2u}1$ | -35.778861 | - | -35.812485 |
| $^1B_{2u}2$ | -34.579035 | - | -34.748219 |
| $^1B_{2u}3$ | -33.635636 | - | -33.753580 |
| $^1B_{1g}1$ | -35.344285 | - | -35.501284 |
| $^1B_{1g}2$ | -34.584524 | - | -34.697143 |
| $^1B_{1g}3$ | -34.106975 | - | -34.336882 |
| $^3B_{3u}1$ | -35.687619 | - | -35.720356 |
| $^3B_{3u}2$ | -34.962464 | - | -35.172472 |

| | | | |
|---|---|---|---|
| $^3B_{3u}3$ | -34.566526 | - | -34.661172 |
| $^3B_{2u}1$ | -37.637311 | - | -37.681022 |
| $^3B_{2u}2$ | -35.721548 | - | -35.830303 |
| $^3B_{2u}3$ | -34.689735 | - | -34.760396 |
| $^3B_{1g}1$ | -36.575920 | - | -36.654869 |
| $^3B_{1g}2$ | -35.223111 | - | -35.350745 |
| $^3B_{1g}3$ | -34.817036 | - | -34.894804 |

Table 6: Acene 4 screened

| State | QCI | FCI | DMRG |
|---|---|---|---|
| $^1A_g1$ | -43.803425 | - | -43.819633 |
| $^1A_g2$ | -40.480116 | - | -40.630868 |
| $^1A_g3$ | -39.508265 | - | -39.605234 |
| $^1B_{3u}1$ | -40.644521 | - | -40.741480 |
| $^1B_{3u}2$ | -39.628651 | - | -39.770199 |
| $^1B_{3u}3$ | -38.804072 | - | -38.883044 |
| $^1B_{2u}1$ | -40.645184 | - | -40.664837 |
| $^1B_{2u}2$ | -39.328619 | - | -39.404653 |
| $^1B_{2u}3$ | -38.767262 | - | -38.812704 |
| $^1B_{1g}1$ | -40.111234 | - | -40.202885 |
| $^1B_{1g}2$ | -39.629159 | - | -39.676013 |
| $^1B_{1g}3$ | -38.885183 | - | -39.003470 |
| $^1B_{3u}1$ | -40.518340 | - | -40.540541 |
| $^1B_{3u}2$ | -39.700907 | - | -39.696836 |
| $^1B_{3u}3$ | -39.654635 | - | -39.804141 |
| $^1B_{2u}1$ | -42.548638 | - | -42.568540 |
| $^1B_{2u}2$ | -40.553948 | - | -40.594250 |
| $^1B_{2u}3$ | -39.306952 | - | -39.338007 |
| $^1B_{1g}1$ | -41.443346 | - | -41.483672 |
| $^1B_{1g}2$ | -40.070842 | - | -40.126336 |
| $^1B_{1g}3$ | -39.480470 | - | -39.516228 |

Table 7: Acene 4 standard

| State | QCI | FCI | DMRG |
|---|---|---|---|
| $^1A_g1$ | -47.439448 | - | -47.348891 |
| $^1A_g2$ | -44.699563 | - | -44.910479 |
| $^1A_g3$ | -43.786253 | - | -43.820491 |
| $^1B_{3u}1$ | -44.418602 | - | -44.466110 |
| $^1B_{3u}2$ | -43.895384 | - | -44.053536 |
| $^1B_{3u}3$ | -43.085336 | - | -43.261614 |
| $^1B_{2u}1$ | -44.793029 | - | -44.850664 |
| $^1B_{2u}2$ | -43.625762 | - | -43.612817 |
| $^1B_{2u}3$ | -42.810721 | - | -42.849819 |
| $^1B_{1g}1$ | -44.378307 | - | -44.385828 |
| $^1B_{1g}2$ | -43.706349 | - | -43.800611 |
| $^1B_{1g}3$ | -42.958385 | - | -42.990826 |
| $^3B_{3u}1$ | -44.495259 | - | -44.458399 |
| $^3B_{3u}2$ | -43.962115 | - | -43.922352 |

| | | | |
|---|---|---|---|
| $^3B_{3u}3$ | -43.279726 | - | -43.364010 |
| $^3B_{2u}1$ | -46.509518 | - | -46.496906 |
| $^3B_{2u}2$ | -44.741928 | - | -44.685572 |
| $^3B_{2u}3$ | -43.804759 | - | -43.694951 |
| $^3B_{1g}1$ | -45.572786 | - | -45.520103 |
| $^3B_{1g}2$ | -44.053453 | - | -43.928040 |
| $^3B_{1g}3$ | -43.911375 | - | -44.020286 |

Table 8: Acene 5 screened

| State | QCI | FCI | DMRG |
|---|---|---|---|
| $^1A_g1$ | -53.613853 | - | -53.580862 |
| $^1A_g2$ | -50.726761 | - | -50.774226 |
| $^1A_g3$ | -49.776017 | - | -49.685725 |
| $^1B_{3u}1$ | -50.471239 | - | -50.541516 |
| $^1B_{3u}2$ | -49.985687 | - | -50.110487 |
| $^1B_{3u}3$ | -48.926640 | - | -48.898681 |
| $^1B_{2u}1$ | -50.754803 | - | -50.736054 |
| $^1B_{2u}2$ | -49.604837 | - | -49.640102 |
| $^1B_{2u}3$ | -49.062026 | - | -49.049947 |
| $^1B_{1g}1$ | -50.314501 | - | -50.381751 |
| $^1B_{1g}2$ | -49.866741 | - | -49.875926 |
| $^1B_{1g}3$ | -48.929835 | - | -48.990156 |
| $^3B_{3u}1$ | -50.522623 | - | -50.508332 |
| $^3B_{3u}2$ | -49.965294 | - | -49.989021 |
| $^3B_{3u}3$ | -49.526575 | - | -49.543904 |
| $^3B_{2u}1$ | -52.625715 | - | -52.598700 |
| $^3B_{2u}2$ | -50.828884 | - | -50.788176 |
| $^3B_{2u}3$ | -49.839179 | - | -49.761629 |
| $^3B_{1g}1$ | -51.664316 | - | -51.654214 |
| $^3B_{1g}2$ | -50.106987 | - | -50.083823 |
| $^3B_{1g}3$ | -49.740003 | - | -49.739688 |

Table 9: Acene 5 standard

## 3.3 Poly-para-phenylenes

| State | QCI | FCI | DMRG |
|---|---|---|---|
| $^1A_g1$ | -25.276600 | -25.300598 | -25.301922 |
| $^1A_g2$ | -20.273411 | -20.444224 | -20.454111 |
| $^1A_g3$ | -19.389983 | -19.524614 | -19.531271 |
| $^1B_{3u}1$ | -20.439358 | -20.451774 | -20.463531 |
| $^1B_{3u}2$ | -19.517546 | -19.675523 | -19.686827 |
| $^1B_{3u}3$ | -19.101009 | -19.164794 | -19.172687 |
| $^1B_{2u}1$ | -21.566103 | -21.691953 | -21.697363 |
| $^1B_{2u}2$ | -19.548886 | -19.729861 | -19.737265 |
| $^1B_{2u}3$ | -19.504499 | -19.573526 | -19.577158 |
| $^1B_{1g}1$ | -21.558152 | -21.684369 | -21.689813 |
| $^1B_{1g}2$ | -19.587761 | -19.731522 | -19.738876 |

| | | | |
|---|---|---|---|
| $^1B_{1g}3$ | -19.547637 | -19.652263 | -19.655780 |
| $^3B_{3u}1$ | -22.697690 | -22.744708 | -22.774956 |
| $^3B_{3u}2$ | -21.546662 | -21.651000 | -21.670490 |
| $^3B_{3u}3$ | -20.262243 | -20.417351 | -20.437279 |
| $^3B_{2u}1$ | -21.544172 | -21.640695 | -21.646954 |
| $^3B_{2u}2$ | -20.191334 | -20.347568 | -20.360260 |
| $^3B_{2u}3$ | -20.091033 | -20.140019 | -20.143288 |
| $^3B_{1g}1$ | -21.543044 | -21.639962 | -21.646144 |
| $^3B_{1g}2$ | -20.193393 | -20.349866 | -20.362482 |
| $^3B_{1g}3$ | -20.076535 | -20.125969 | -20.129165 |

Table 10: PPP 2 screened

| State | QCI | FCI | DMRG |
|---|---|---|---|
| $^1A_g1$ | -28.760137 | -28.767592 | -28.767843 |
| $^1A_g2$ | -23.136526 | -23.169327 | -23.171134 |
| $^1A_g3$ | -23.025073 | -23.091050 | -23.093474 |
| $^1B_{3u}1$ | -23.942720 | -23.949888 | -23.952034 |
| $^1B_{3u}2$ | -22.551390 | -22.574648 | -22.578527 |
| $^1B_{3u}3$ | -22.280368 | -22.336187 | -22.339850 |
| $^1B_{2u}1$ | -24.657019 | -24.700708 | -24.701933 |
| $^1B_{2u}2$ | -22.225087 | -22.299529 | -22.301822 |
| $^1B_{2u}3$ | -22.126667 | -22.155062 | -22.156559 |
| $^1B_{1g}1$ | -24.628540 | -24.671927 | -24.673159 |
| $^1B_{1g}2$ | -22.481176 | -22.506186 | -22.507420 |
| $^1B_{1g}3$ | -22.227387 | -22.300490 | -22.302733 |
| $^3B_{3u}1$ | -25.636474 | -25.651992 | -25.660784 |
| $^3B_{3u}2$ | -24.618959 | -24.653179 | -24.658258 |
| $^3B_{3u}3$ | -23.156156 | -23.207588 | -23.213357 |
| $^3B_{2u}1$ | -24.590236 | -24.621085 | -24.622506 |
| $^3B_{2u}2$ | -23.472804 | -23.487676 | -23.488463 |
| $^3B_{2u}3$ | -23.013011 | -23.067811 | -23.071959 |
| $^3B_{1g}1$ | -24.589162 | -24.620097 | -24.621416 |
| $^3B_{1g}2$ | -23.434095 | -23.449511 | -23.450247 |
| $^3B_{1g}3$ | -23.019234 | -23.074266 | -23.078284 |

Table 11: PPP 2 standard

| State | QCI | FCI | DMRG |
|---|---|---|---|
| $^1A_g1$ | -38.203416 | - | -38.270704 |
| $^1A_g2$ | -33.517632 | - | -33.909513 |
| $^1A_g3$ | -32.631245 | - | -32.962799 |
| $^1B_{3u}1$ | -33.917761 | - | -34.022909 |
| $^1B_{3u}2$ | -32.886434 | - | -33.287118 |
| $^1B_{3u}3$ | -32.108854 | - | -32.412953 |
| $^1B_{2u}1$ | -34.392208 | - | -34.566265 |
| $^1B_{2u}2$ | -34.202920 | - | -34.773265 |
| $^1B_{2u}3$ | -32.587193 | - | -32.832918 |
| $^1B_{1g}1$ | -34.155958 | - | -34.566200 |
| $^1B_{1g}2$ | -32.542788 | - | -32.833733 |
| $^1B_{1g}3$ | -32.485042 | - | -32.824832 |
| $^3B_{3u}1$ | -35.687638 | - | -35.881183 |
| $^3B_{3u}2$ | -34.683248 | - | -35.058415 |

| | | | |
|---|---|---|---|
| $^3B_{3u}3$ | -34.306740 | - | -34.665373 |
| $^3B_{2u}1$ | -34.395798 | - | -34.494016 |
| $^3B_{2u}2$ | -34.224587 | - | -34.701800 |
| $^3B_{2u}3$ | -33.129854 | - | -33.353631 |
| $^3B_{1g}1$ | -34.182725 | - | -34.494144 |
| $^3B_{1g}2$ | -33.173001 | - | -33.217804 |
| $^3B_{1g}3$ | -32.896993 | - | -33.166982 |

Table 12: PPP 3 screened

| State | QCI | FCI | DMRG |
|---|---|---|---|
| $^1A_g1$ | -43.450717 | - | -43.471272 |
| $^1A_g2$ | -38.121553 | - | -38.276099 |
| $^1A_g3$ | -38.097122 | - | -38.244591 |
| $^1B_{3u}1$ | -39.021531 | - | -39.066661 |
| $^1B_{3u}2$ | -37.734200 | - | -37.831553 |
| $^1B_{3u}3$ | -37.527501 | - | -37.683912 |
| $^1B_{2u}1$ | -39.349500 | - | -39.509281 |
| $^1B_{2u}2$ | -39.194809 | - | -39.349549 |
| $^1B_{2u}3$ | -37.248064 | - | -37.384462 |
| $^1B_{1g}1$ | -39.179264 | - | -39.350968 |
| $^1B_{1g}2$ | -36.996591 | - | -37.148503 |
| $^1B_{1g}3$ | -36.984715 | - | -37.089500 |
| $^3B_{3u}1$ | -40.476097 | - | -40.548155 |
| $^3B_{3u}2$ | -39.573657 | - | -39.716053 |
| $^3B_{3u}3$ | -39.246475 | - | -39.389047 |
| $^3B_{2u}1$ | -39.304023 | - | -39.269880 |
| $^3B_{2u}2$ | -39.170955 | - | -39.428875 |
| $^3B_{2u}3$ | -38.273008 | - | -38.361988 |
| $^3B_{1g}1$ | -39.153565 | - | -39.269825 |
| $^3B_{1g}2$ | -38.076551 | - | -38.171140 |
| $^3B_{1g}3$ | -37.813777 | - | -38.031123 |

Table 13: PPP 3 standard

## 3.4 Trigonal zigzag graphene nanodisks

| System | Parameters | $A_1$ | $B_2$ |
|---|---|---|---|
| TZGND-1 doublet | Screened | -25.784324 | -27.793568 |
| | | -25.366065 | -25.786939 |
| | | -24.404038 | -24.409357 |
| | Standard | -29.160049 | -31.379637 |
| | | -28.728226 | -29.160574 |
| | | -27.792477 | -27.635932 |
| TZGND-2 singlet | Screened | -47.682268 | -47.682346 |
| | | -45.908450 | -45.907757 |
| | | -45.596365 | -45.596343 |
| | Standard | -53.830723 | -53.830848 |
| | | -51.876156 | -51.876491 |
| | | -51.559202 | -51.559564 |
| TZGND-2 triplet | Screened | -45.922645 | -48.201089 |
| | | -45.764165 | -46.057782 |
| | | -45.441111 | -45.841121 |
| | Standard | -52.021886 | -54.359609 |
| | | -51.804331 | -52.081932 |
| | | -51.520589 | -51.847026 |

Table 14: TZGND gound and excited state DMRG energies