**기존 데이터.**

**Table 5.** Energy of Dimer for each Ansatz/Optimizer for each Oxidation State of

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| [x=1] | UCCSD | | | Two-Local | | |
| Configuration | COBYLA | SPSA | L-BFGS-B | COBYLA | SPSA | L-BFGS-B |
| “Li-O1” | -81.036530 | -81.062982 | -81.069739 | -81.023626 | -80.978418 | -81.069703 |
| “Li-O2” | -81.117531 | -81.117951 | -81.117956 | -81.094238 | -81.030553 | -81.117577 |
| “Li-Co” | -1373.429758 | -1373.567946 | -1373.618739 | -1373.576316 | -1373.512522 | -1373.609970 |
| “O-O” | -147.432250 | -147.485749 | -147.599156 | -147.528891 | -147.334234 | -147.605860 |
| “Co-O1” | -1439.355819 | -1439.796790 | -1439.957262 | -1439.315189 | -1439.321781 | -1439.695408 |
| “Co-O2” | -1439.459214 | -1439.788926 | -1439.888880 | -1439.396154 | -1439.727786 | -1439.918488 |
| [x=0.94] | UCCSD | | | Two-Local | | |
| Configuration | COBYLA | SPSA | L-BFGS-B | COBYLA | SPSA | L-BFGS-B |
| “Li-O1” | -81.079066 | -81.071382 | -81.084085 | -81.014315 | -81.042272 | -81.084060 |
| “Li-O2” | -81.119992 | -81.119699 | -81.120071 | -81.117758 | -81.066772 | -81.120071 |
| “Li-Co” | -1373.434678 | -1373.568648 | -1373.569509 | -1373.347301 | -1373.529010 | -1373.584236 |
| “O-O” | -147.391974 | -147.374393 | -147.608042 | -147.551759 | -147.523597 | -147.489992 |
| “Co-O1” | -1439.423661 | -1439.843317 | -1439.952027 | -1439.169880 | -1439.485884 | -1439.803393 |
| “Co-O2” | -1439.393635 | -1439.485720 | -1439.898848 | -1439.210821 | -1439.564247 | -1439.986058 |
| [x=0.78] | UCCSD | | | Two-Local | | |
| Configuration | COBYLA | SPSA | L-BFGS-B | COBYLA | SPSA | L-BFGS-B |
| “Li-O1” | -81.074588 | -81.076294 | -81.086310 | -81.070688 | -81.021452 | -81.086299 |
| “Li-O2” | -81.118325 | -81.119637 | -81.120088 | -81.097025 | -81.058402 | -81.119684 |
| “Li-Co” | -1373.206240 | -1373.319480 | -1373.354329 | -1373.591995 | -1373.380891 | -1373.725492 |
| “O-O” | -147.412124 | -147.551726 | -147.607067 | -147.517407 | -147.166796 | -147.560823 |
| “Co-O1” | -1439.226044 | -1439.778362 | -1439.840047 | -1439.319849 | -1439.523202 | -1439.714842 |
| “Co-O2” | -1439.547179 | -1439.828032 | -1439.944688 | -1439.300309 | -1439.408856 | -1439.738547 |
| [x=0.75] | UCCSD | | | Two-Local | | |
| Configuration | COBYLA | SPSA | L-BFGS-B | COBYLA | SPSA | L-BFGS-B |
| “Li-O1” | -81.065682 | -81.081421 | -81.086310 | -81.003117 | -81.023070 | -81.012210 |
| “Li-O2” | -81.119826 | -81.120074 | -81.120088 | -81.095257 | -81.071903 | -81.120088 |
| “Li-Co” | -1373.223660 | -1373.354256 | -1373.328463 | -1373.589681 | -1373.585003 | -1373.790507 |
| “O-O” | -147.413053 | -147.281268 | -147.607526 | -147.445853 | -147.442307 | -147.462992 |
| “Co-O1” | -1439.226044 | -1439.778362 | -1439.840047 | -1439.319849 | -1439.523202 | -1439.714842 |
| “Co-O2” | -1439.388348 | -1439.758178 | -1439.857075 | -1439.354511 | -1439.479002 | -1439.722998 |
| [x=0.66] | UCCSD | | | Two-Local | | |
| Configuration | COBYLA | SPSA | L-BFGS-B | COBYLA | SPSA | L-BFGS-B |
| “Li-O1” | -81.053296 | -80.984815 | -81.084085 | -81.014315 | -81.042272 | -81.084060 |
| “Li-O2” | -81.119992 | -81.119699 | -81.120071 | -81.117758 | -81.066772 | -81.120071 |
| “Li-Co” | -1373.434678 | -1373.568648 | -1373.569509 | -1373.347301 | -1373.529010 | -1373.584236 |
| “O-O” | -147.391974 | -147.374393 | -147.608042 | -147.551759 | -147.523597 | -147.489992 |
| “Co-O1” | -1439.423661 | -1439.843317 | -1439.952027 | -1439.169880 | -1439.485884 | -1439.803393 |
| “Co-O2” | -1439.393635 | -1439.485720 | -1439.898848 | -1439.210821 | -1439.564247 | -1439.986058 |

텍스트, 라인, 도표, 그래프이(가) 표시된 사진

자동 생성된 설명라인, 텍스트, 도표, 그래프이(가) 표시된 사진

자동 생성된 설명

**Table 5.** Comparison of the energy, error, and accuracy between FMO/VQE and FCI.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Oxidation  Number  () |  |  | Error | Accuracy(%) |
| 1.00 | -1521.203868 | -1521.244330 | 0.040462 | 99.9973 |
| 0.94 | -1521.250344 | -1521.244451 | -0.005892 | 99.9996 |
| 0.78 | -1521.239517 | -1521.247824 | 0.008307 | 99.9995 |
| 0.75 | -1521.217377 | -1521.248807 | 0.031431 | 99.9979 |
| 0.66 | -1521.163133 | -1521.249196 | 0.086063 | 99.9943 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Oxidation  Number  () |  |  | Error | Accuracy(%) |
| 1.00 | -1521.203868 | -1521.342101 | 0.138232 | 99.9884 |
| 0.94 | -1521.250344 | -1521.338869 | 0.088525 | 99.9919 |
| 0.78 | -1521.239517 | -1521.341358 | 0.101841 | 99.9933 |
| 0.75 | -1521.217377 | -1521.340712 | 0.123336 | 99.9942 |
| 0.66 | -1521.163133 | -1521.340283 | 0.177150 | 99.9909 |

**새로운 데이터**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| [x=1] | UCCSD | | | Two-Local | | |
| Configuration | COBYLA | SPSA | L-BFGS-B | COBYLA | SPSA | L-BFGS-B |
| “Li-O1” | -81.036530 | -81.062982 | -81.069739 | -81.023626 | -80.978418 | -81.069703 |
| “Li-O2” | -81.117531 | -81.117951 | -81.117956 | -81.094238 | -81.030553 | -81.117577 |
| “Li-Co” | -1373.429758 | -1373.567946 | -1373.618739 | -1373.576316 | -1373.512522 | -1373.609970 |
| “O-O” | -147.432250 | -147.485749 | -147.599156 | -147.528891 | -147.334234 | -147.605860 |
| “Co-O1” | -1439.355819 | -1439.796790 | -1439.957262 | -1439.315189 | -1439.321781 | -1439.695408 |
| “Co-O2” | -1439.459214 | -1439.788926 | -1439.888880 | -1439.396154 | -1439.727786 | -1439.918488 |
| [x=0.94] | UCCSD | | | Two-Local | | |
| Configuration | COBYLA | SPSA | L-BFGS-B | COBYLA | SPSA | L-BFGS-B |
| “Li-O1” | -81.079066 | -81.071382 | -81.084085 | -81.014315 | -81.042272 | -81.084060 |
| “Li-O2” | -81.119992 | -81.119699 | -81.120071 | -81.117758 | -81.066772 | -81.120071 |
| “Li-Co” | -1373.434678 | -1373.568648 | -1373.569509 | -1373.347301 | -1373.529010 | -1373.584236 |
| “O-O” | -147.391974 | -147.374393 | -147.608042 | -147.551759 | -147.523597 | -147.489992 |
| “Co-O1” | -1439.423661 | -1439.843317 | -1439.952027 | -1439.169880 | -1439.485884 | -1439.803393 |
| “Co-O2” | -1439.393635 | -1439.485720 | -1439.898848 | -1439.210821 | -1439.564247 | -1439.986058 |
| [x=0.78] | UCCSD | | | Two-Local | | |
| Configuration | COBYLA | SPSA | L-BFGS-B | COBYLA | SPSA | L-BFGS-B |
| “Li-O1” | -81.074588 | -81.076294 | -81.086310 | -81.070688 | -81.021452 | -81.086299 |
| “Li-O2” | -81.118325 | -81.119637 | -81.120088 | -81.097025 | -81.058402 | -81.119684 |
| “Li-Co” | -1373.206240 | -1373.319480 | -1373.354329 | -1373.591995 | -1373.380891 | -1373.725492 |
| “O-O” | -147.412124 | -147.551726 | -147.607067 | -147.517407 | -147.166796 | -147.560823 |
| “Co-O1” | -1439.226044 | -1439.778362 | -1439.840047 | -1439.319849 | -1439.523202 | -1439.714842 |
| “Co-O2” | -1439.547179 | -1439.828032 | -1439.944688 | -1439.300309 | -1439.408856 | -1439.738547 |
| [x=0.75] | UCCSD | | | Two-Local | | |
| Configuration | COBYLA | SPSA | L-BFGS-B | COBYLA | SPSA | L-BFGS-B |
| “Li-O1” | -81.065682 | -81.081421 | -81.086310 | -81.003117 | -81.023070 | -81.012210 |
| “Li-O2” | -81.119826 | -81.120074 | -81.120088 | -81.095257 | -81.071903 | -81.120088 |
| “Li-Co” | -1373.223660 | -1373.354256 | -1373.328463 | -1373.589681 | -1373.585003 | -1373.790507 |
| “O-O” | -147.413053 | -147.281268 | -147.607526 | -147.445853 | -147.442307 | -147.462992 |
| “Co-O1” | -1439.226044 | -1439.778362 | -1439.840047 | -1439.319849 | -1439.523202 | -1439.714842 |
| “Co-O2” | -1439.388348 | -1439.758178 | -1439.857075 | -1439.354511 | -1439.479002 | -1439.722998 |

* 흑백에서의 가독성 위해 마커 추가.
* X=0.66 에서의 데이터 삭제.

텍스트, 라인, 그래프, 도표이(가) 표시된 사진

AI가 생성한 콘텐츠는 부정확할 수 있습니다.텍스트, 라인, 도표, 그래프이(가) 표시된 사진

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|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Oxidation  Number  () |  |  | Error | Accuracy(%) |
| 1.00 | -1521.203868 | -1521.244330 | 0.040462 | 99.9973 |
| 0.94 | -1521.250344 | -1521.244451 | -0.005892 | 99.9996 |
| 0.78 | -1521.239517 | -1521.247824 | 0.008307 | 99.9995 |
| 0.75 | -1521.217377 | -1521.248807 | 0.031431 | 99.9979 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Oxidation  Number  () |  |  | Error | Accuracy(%) |
| 1.00 | -1521.203868 | -1521.342101 | 0.138232 | 99.9884 |
| 0.94 | -1521.250344 | -1521.338869 | 0.088525 | 99.9919 |
| 0.78 | -1521.239517 | -1521.341358 | 0.101841 | 99.9933 |
| 0.75 | -1521.217377 | -1521.340712 | 0.123336 | 99.9942 |