|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Кнопка | Функція |  |  |
|  |  |  |  |  |
| 1 | import\_out\_button | showDialogRead() |  |  |
|  |  |  |  |  |
| 2 | Export\_AA\_AB\_BB | export\_cation\_cation\_func() |  |  |
| 3 | Export\_AO\_BO | export\_cation\_anion\_func() |  |  |
| 4 | Export\_OO | export\_OO\_func() |  |  |
|  |  |  |  |  |
| 5 | Angle\_B\_B\_B | export\_BBB\_func() |  |  |
| 6 | Angle\_B\_O\_B | export\_BOB\_func() |  |  |
|  |  |  |  |  |
| 7 | ave\_AA | calculate\_ave\_AA\_func() |  |  |
| 8 | ave\_AB | calculate\_ave\_AB\_func() |  |  |
| 9 | ave\_BB | calculate\_ave\_BB\_func() |  |  |
| 10 | ave\_AA\_BB | calculate\_ave\_AABB\_func() |  |  |
|  |  |  |  |  |
| 11 | ave\_AO | calculate\_ave\_AO\_func() |  |  |
| 12 | ave\_BO | calculate\_ave\_BO\_func() |  |  |
| 13 | ave\_OO | calculate\_ave\_OO\_func() |  |  |
| 14 | ave\_Theta | calculate\_ave\_Theta\_func() |  |  |
|  |  |  |  |  |
| 15 | def\_AA | calculate\_def\_AA\_func() |  |  |
| 16 | def\_AB | calculate\_def\_AB\_func() |  |  |
| 17 | def\_BB | calculate\_def\_BB\_func() |  |  |
| 18 | maxmin\_AB | calculate\_maxmin\_AB\_func() |  |  |
|  |  |  |  |  |
| 19 | def\_AO | calculate\_def\_AO\_func() |  |  |
| 20 | def\_BO | calculate\_def\_BO\_func() |  |  |
| 21 | Tolerance | calculate\_tolerance\_func() |  |  |
| 22 | Bandwidth | calculate\_bandwidth\_func() |  |  |
|  |  |  |  |  |
| 23 | Edit\_variables | edit\_variables\_func() |  |  |
| 24 | Save\_variables | save\_variables\_func() |  |  |
|  |  |  |  |  |
| 25 | Edit\_results | edit\_results\_func() |  |  |
| 26 | Save\_results | save\_results\_func() |  |  |
|  |  |  |  |  |
| 27 | export\_to\_file | showDialogWrite() |  |  |

python -m PyQt5.uic.pyuic -x perovskite\_deformation\_with\_signals.ui -o window.py

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| *La1-xPrx* | **0.5** | **0.55** | **0.6** | **0.65** | **0.8** | **Pr** |
| R-2Co1 | 3.199 | 3.194 | 3.193 | 3.184 | 3.1615 | 3.148 |
| R-2Co2 | 3.299 | 3.295 | 3.295 | 3.296 | 3.276 | 3.272 |
| R-2Co3 | 3.324 | 3.323 | 3.32 | 3.314 | 3.321 | 3.309 |
| R-2Co4 | 3.374 | 3.376 | 3.376 | 3.382 | 3.3964 | 3.4 |
| R-Co\_Ave | 3.2990 | 3.2970 | 3.2960 | 3.2940 | 3.2887 | 3.2823 |
| Max/Min | 1.0547 | 1.0570 | 1.0573 | 1.0622 | 1.0743 | 1.0801 |
|  |  |  |  |  |  |  |
| R-2R1 | 3.7886 | 3.7849 | 3.7849 | 3.7889 | 3.7572 | 3.755 |
| R-2R2 | 3.81023 | 3.80854 | 3.80714 | 3.80674 | 3.80411 | 3.799 |
| R-2R3 | 3.8326 | 3.8319 | 3.8289 | 3.8201 | 3.8362 | 3.821 |
| R-R\_Ave | 3.8105 | 3.8084 | 3.8070 | 3.8052 | 3.7992 | 3.7917 |
|  |  |  |  |  |  |  |
| Co-2Co | 3.80402 | 3.80182 | 3.80032 | 3.79892 | 3.79281 | 3.786 |
| Co-4Co | 3.81001 | 3.80772 | 3.80632 | 3.80362 | 3.79611 | 3.788 |
| Co-Co\_Ave | 3.8080 | 3.8058 | 3.8043 | 3.8021 | 3.7950 | 3.7873 |
|  |  |  |  |  |  |  |
| (RR)6/(CoCo)6 | 1.0006 | 1.0007 | 1.0007 | 1.0008 | 1.0011 | 1.0011 |
| D(RCo)8 | 0.3733 | 0.4032 | 0.4047 | 0.4665 | 0.6699 | 0.7590 |
| D(RR)6 | 0.0222 | 0.0254 | 0.0223 | 0.0113 | 0.0729 | 0.0524 |
| D(CoCo)6 | 0.0005 | 0.0005 | 0.0006 | 0.0003 | 0.0002 | 0.0001 |

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| *La1-xPrx* | **0.5** | **0.55** | **0.6** | **0.65** | **0.8** | **Pr** |
| R-1-O1 | 2.393 | 2.424 | 2.263 | 2.314 | 2.285 | 2.358 |
| R-2-O2 | 2.392 | 2.423 | 2.423 | 2.424 | 2.455 | 2.358 |
| R-1-O1 | 2.592 | 2.593 | 2.563 | 2.583 | 2.583 | 2.515 |
| R-2-O2 | 2.572 | 2.623 | 2.623 | 2.654 | 2.595 | 2.588 |
| R-2-O2 | 2.762 | 2.693 | 2.693 | 2.654 | 2.685 | 2.668 |
| R-1-O1 | 2.822 | 2.813 | 2.863 | 2.843 | 2.833 | 2.879 |
| R-1-O1 | 3.043 | 3.004 | 3.163 | 3.104 | 3.115 | 3.029 |
| R-2-O2 | 3.102 | 3.083 | 3.083 | 3.084 | 3.065 | 3.134 |
| (RO)8 | 2.5546 | 2.5619 | 2.5380 | 2.5451 | 2.5423 | 2.5126 |
| (RO)9 | 2.5843 | 2.5898 | 2.5741 | 2.5782 | 2.5746 | 2.5533 |
| (RO)10 | 2.6302 | 2.6312 | 2.6330 | 2.6308 | 2.6286 | 2.6009 |
| (RO)12 | 2.7088 | 2.7065 | 2.7080 | 2.7063 | 2.7013 | 2.6898 |
|  |  |  |  |  |  |  |
| Co-2-O2 | 1.833 | 1.933 | 1.893 | 1.874 | 1.886 | 1.928 |
| Co-2-O1 | 1.9325 | 1.9266 | 1.9497 | 1.9438 | 1.94311 | 1.927 |
| Co-2-O2 | 2.043 | 1.944 | 1.983 | 1.993 | 1.965 | 1.929 |
| (CoO)6 | 1.9362 | 1.9345 | 1.9419 | 1.9369 | 1.9314 | 1.9280 |
| t8 | 0.9330 | 0.9364 | 0.9242 | 0.9291 | 0.9308 | 0.9215 |
| t9 | 0.9438 | 0.9466 | 0.9373 | 0.9412 | 0.9426 | 0.9365 |
| t10 | 0.9606 | 0.9618 | 0.9588 | 0.9604 | 0.9624 | 0.9539 |
| t12 | 0.9893 | 0.9893 | 0.9861 | 0.9880 | 0.9890 | 0.9865 |
|  |  |  |  |  |  |  |
| Co-01-Co |  |  |  |  |  |  |
| Co-02-Co |  |  |  |  |  |  |
| ThetaZ | 90 | 90 | 90 | 90 | 90 | 90 |
| ThetaY | 90 | 90 | 90 | 90 | 90 | 90 |
| ThetAve | 90 | 90 | 90 | 90 | 90 | 90 |
|  |  |  |  |  |  |  |
| O2-2-O2 | 2.683 | 2.695 | 2.704 | 2.716 | 2.687 | 2.692 |
| O2-1-O1 | 2.633 | 2.704 | 2.634 | 2.674 | 2.646 | 2.709 |
| O2-1\*O1 | 2.703 | 2.724 | 2.714 | 2.714 | 2.746 | 2.726 |
| O2-1-O1 | 2.773 | 2.724 | 2.794 | 2.724 | 2.777 | 2.726 |
| O2-1\*O1 | 2.853 | 2.764 | 2.844 | 2.855 | 2.786 | 2.744 |
| O2-2\*O2 | 2.814 | 2.775 | 2.774 | 2.755 | 2.768 | 2.763 |
| (O2-O2)ave | 2.7485 | 2.7350 | 2.7390 | 2.7355 | 2.7275 | 2.7275 |
| (O2-O1)ave | 2.7405 | 2.7290 | 2.7465 | 2.7418 | 2.7388 | 2.7263 |
| (OO)8 | 2.7445 | 2.7320 | 2.7428 | 2.7386 | 2.7331 | 2.7269 |
|  |  |  |  |  |  |  |
| D(RO)8 | 3.1992 | 1.9124 | 3.2058 | 2.5397 | 2.5024 | 2.6012 |
| D(RO)9 | 3.8359 | 2.5921 | 4.3446 | 3.5183 | 3.4285 | 4.2725 |
| D(RO)10 | 6.0699 | 4.4905 | 8.2392 | 6.6359 | 6.7645 | 6.7162 |
| D(RO)12 | 8.9821 | 7.4071 | 10.3262 | 9.1204 | 8.9624 | 10.6890 |
|  |  |  |  |  |  |  |
| D(CoO)6 | 1.96245 | 0.01380 | 0.36606 | 0.63537 | 0.29733 | 0.00018 |