Scripts summary

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| --- | --- | --- | --- | --- |
| **Script name** | **Path to script** | **input** | **output** | **Notes** |
| logdata.py | /blue/mingjieliu/adrian.gonzalezs/scripts | \*.log | data.csv | Get HOMO, LUMO, HF, RMSD, RMSF, Dipole |
| movefail.py | /blue/mingjieliu/adrian.gonzalezs/scripts | folder | folder | Moves all failed jobs to a folder named ‘failed’ in the same directory. If file already exists will add a number to file name. |
| distancematrix.py | /blue/mingjieliu/wangzhiyu/script | \*.xyz | value | Read xyz, get spefic atom position |
| distancematrix.py | /blue/mingjieliu/wangzhiyu/script | \*.xyz | distance\_matrix.txt | Read batch of xyz and list structure and distance in two columns |
| job\_done.py | /blue/mingjieliu/wangzhiyu/script | folder | folder | Extract normal termination job to a separate folder |
| global\_curvature.py | /blue/mingjieliu/wangzhiyu/script | \*xyz | .dat/.pdf | Calculate and plot z axis difference of substrate to represent golocal curvature |
| local\_curvature.py | /blue/mingjieliu/wangzhiyu/script | \*xyz | .dat | Calculate z axis value difference of single atom |
| extract\_coor\_orignal.py | /blue/mingjieliu/wangzhiyu/script | \*log | .xyz | Extract original structure |
| extract\_coor\_opt.py | /blue/mingjieliu/wangzhiyu/script | \*log | .xyz | Extract optimized structure |
| all\_submit.py | /blue/mingjieliu/wangzhiyu/script | \*xyz | .com/.sh | Write input, generate directory,job submission, charge calculation input in one script .(need to combine with chain.sh to submit dependent job) |
| metal\_position.py | /blue/mingjieliu/wangzhiyu/script | \*xyz | .dat | Read optimized xyz file and represent postion of certain element by summing over all distance to outermost hydrogen |
| avg\_bl.py | /blue/mingjieliu/wangzhiyu/script | .xyz | .dat | Get average bond length around single atom |
| bader\_charge.sh | /blue/mingjieliu/wangzhiyu/script | \*chk | \*dat | Generate bader charge in ACF.dat |
| j1.sh | /blue/mingjieliu/wangzhiyu/script | \*wfx | \*xyz | Generate DDEC6 charge in a xyz file |
| extract\_table\_for\_natural\_charge.py | /blue/mingjieliu/wanghongyi | \*log | \*txt | Create NBO analysis table including NBO charge |
| get\_structures.py | /blue/mingjieliu/so.farajinafchi/scripts | \*log  \*xyz | \*xyz | Extracts all the structures during the geometry optimization |

Extract properties from .log:

|  |  |  |
| --- | --- | --- |
| Property | Name | Unit |
| Job status (success or fail) | Job\_stat | (S/F, or error msg?) |
| Basis sets | basis\_sets |  |
| Functional | functional |  |
| Spin multiplicity | spin\_multi |  |
| Total charge | total\_chg |  |
| Stoichiometry | stoichiometry |  |
| Spin\_opt, <s2> ie. (S(S+1)) | S2 |  |
| time |  |  |
| # of cpu | Nproc |  |
| Electronic energy | E\_HF | Hartree |
| HOMO | HOMO | Hartree |
| LUMO | LUMO | Hartree |
| HOMO-LUMO gap | HOMO\_LUMO\_gap | eV |
| Mulliken charge | Mulliken | (.dat) |
| Hirshfeld charge | Hirshfeld | (.dat) |
| CM5 charge | CM5 | (.dat) |
| NBO charge | NBO\_charge | (.dat) |
| Dipole moment | Dip\_tot |  |
| Dipole moment xyz | Dip\_x, Dip\_y, Dip\_z |  |
| Initial geometry | Ini\_geo | (.xyz file) |
| Optimized geometry | Opt\_geo | (.xyz file) |
| RMSD | RMSD |  |
| RMSF | RMSD |  |