Duplicates

```
>>> len(adE_OH)
3060
>>> len(OH_duplicates1)
28
>>> len(OH_duplicates2)
24
>>> len(OH_duplicates3)
692
>>> len(adE_OH3)
2316
>>> 3060 - 28 - 24 - 692
2316
```

```
>>> len(adE_O)
7996
>>> len(O_duplicates1)
1051
>>> len(O_duplicates2)
1702
>>> len(O_duplicates3)
1666
>>> len(adE_O3)
3577
>>> 7996 - 1051 - 1702 - 1666
3577
```

```
>>> len(adE_OOH)
3238
>>> len(OOH_duplicates1)
68
>>> len(OOH_duplicates3)
791
>>> len(adE_OOH3)
2379
>>> 3238 - 68 -791
2379
```

```
>>> OH_duplicates1
          bulk_id miller_index  nads bulk_symbols  slab_sid ads_symbols  adsorption_energy       diff
system_id
3073      mp-1180693   (0, 1, 0)     1     Li2Se4O12     26410          OH           0.417874        NaN
8862      mp-1180693   (0, 1, 0)     1     Li2Se4O12     26410          OH           0.054306   0.363568
>>> adE.loc[3073]
bulk_id              mp-1180693
miller_index          (0, 1, 0)
nads                          1
bulk_symbols          Li2Se4O12
slab_sid                  26410
ads_symbols                  OH
adsorption_energy      0.417874
Name: 3073, dtype: object
>>> adE.loc[8862]
bulk_id              mp-1180693
miller_index          (0, 1, 0)
nads                          1
bulk_symbols          Li2Se4O12
slab_sid                  26410
ads_symbols                  OH
adsorption_energy      0.054306
Name: 8862, dtype: object
>>> 0.417874 - 0.054306
0.363568
```

```
>>> OH_duplicates2
   system_id     bulk_id miller_index  nads bulk_symbols  slab_sid ads_symbols  adsorption_energy       diff
0      15546  mp-1183405   (1, 1, 0)     1     Ba1Zn1O3     19468          OH          -0.036996        NaN
1      12088  mp-1183405   (1, 1, 0)     3     Ba1Zn1O3     19468          OH           0.570337   0.607334

>>> adE_OH.loc[15546]
bulk_id              mp-1183405
miller_index          (1, 1, 0)
nads                          1
bulk_symbols           Ba1Zn1O3
slab_sid                  19468
ads_symbols                  OH
adsorption_energy     -0.036996
Name: 15546, dtype: object
>>> adE_OH.loc[12088]
bulk_id              mp-1183405
miller_index          (1, 1, 0)
nads                          3
bulk_symbols           Ba1Zn1O3
slab_sid                  19468
ads_symbols                  OH
adsorption_energy      0.570337
Name: 12088, dtype: object
>>> 0.570337 + 0.036996
0.607333
```

```
>>> OH_duplicates3
                bulk_id miller_index  nads bulk_symbols  slab_sid ads_symbols  adsorption_energy      diff
system_id
29734      AgSbO4-rutile    (2, 1, 1)     4     Ag1Sb1O4     24300          OH           0.560136       NaN
41675      AgSbO4-rutile    (2, 1, 1)     2     Ag1Sb1O4     42864          OH           1.457995  0.897860
>>> adE_OH.loc[29734]
bulk_id                AgSbO4-rutile
miller_index               (2, 1, 1)
nads                               4
bulk_symbols                Ag1Sb1O4
slab_sid                       24300
ads_symbols                       OH
adsorption_energy           0.560136
Name: 29734, dtype: object
>>> adE_OH.loc[41675]
bulk_id                AgSbO4-rutile
miller_index               (2, 1, 1)
nads                               2
bulk_symbols                Ag1Sb1O4
slab_sid                       42864
ads_symbols                       OH
adsorption_energy           1.457995
Name: 41675, dtype: object
>>> 1.457995 - 0.560136
0.897859
```

```
>>> O_duplicates1
                bulk_id miller_index  nads bulk_symbols  slab_sid ads_symbols  adsorption_energy      diff
system_id
24729      AgIrO4-rutile    (2, 1, 3)     2     Ag1Ir1O4     34579           O           2.597050       NaN
29995      AgIrO4-rutile    (2, 1, 3)     2     Ag1Ir1O4     34579           O           2.051319  0.545730
>>> adE_O.loc[24729]
bulk_id                AgIrO4-rutile
miller_index               (2, 1, 3)
nads                               2
bulk_symbols                Ag1Ir1O4
slab_sid                       34579
ads_symbols                        O
adsorption_energy            2.59705
Name: 24729, dtype: object
>>> adE_O.loc[29995]
bulk_id                AgIrO4-rutile
miller_index               (2, 1, 3)
nads                               2
bulk_symbols                Ag1Ir1O4
slab_sid                       34579
ads_symbols                        O
adsorption_energy           2.051319
Name: 29995, dtype: object
>>> 2.59705 - 2.051319
0.545731
```

```
>>> O_duplicates2
             bulk_id miller_index  nads bulk_symbols  slab_sid ads_symbols  adsorption_energy      diff
system_id
20832      AgRhO4-rutile    (1, 0, 1)     2      Ag1Rh1O4     80231           O           3.058531       NaN
19873      AgRhO4-rutile    (1, 0, 1)     3      Ag1Rh1O4     80231           O           2.252256  0.806275
>>> adE_O.loc[20832]
bulk_id               AgRhO4-rutile
miller_index              (1, 0, 1)
nads                              2
bulk_symbols               Ag1Rh1O4
slab_sid                      80231
ads_symbols                       O
adsorption_energy          3.058531
Name: 20832, dtype: object
>>> adE_O.loc[19873]
bulk_id               AgRhO4-rutile
miller_index              (1, 0, 1)
nads                              3
bulk_symbols               Ag1Rh1O4
slab_sid                      80231
ads_symbols                       O
adsorption_energy          2.252256
Name: 19873, dtype: object
>>> 3.058531 - 2.252256
0.8062749999999999
```

```
>>> O_duplicates3
             bulk_id miller_index  nads bulk_symbols  slab_sid ads_symbols  adsorption_energy      diff
system_id
44742      AgHgO4-rutile    (1, 1, 0)     4      Ag1Hg1O4     41568           O           2.516844       NaN
43443      AgHgO4-rutile    (1, 1, 0)     2      Ag1Hg1O4     44232           O           2.519054  0.002210
>>> adE.loc[44742]
bulk_id               AgHgO4-rutile
miller_index              (1, 1, 0)
nads                              4
bulk_symbols               Ag1Hg1O4
slab_sid                      41568
ads_symbols                       O
adsorption_energy          2.516844
Name: 44742, dtype: object
>>> adE.loc[43443]
bulk_id               AgHgO4-rutile
miller_index              (1, 1, 0)
nads                              2
bulk_symbols               Ag1Hg1O4
slab_sid                      44232
ads_symbols                       O
adsorption_energy          2.519054
Name: 43443, dtype: object
>>> 2.519054 - 2.516844
0.0022100000000002673
```

```
>>> OOH_duplicates1
           bulk_id miller_index  nads bulk_symbols  slab_sid ads_symbols  adsorption_energy      diff
system_id
12100    mp-1262087    (0, 1, 0)     1   Al4Bi12O36      8090         HO2           3.425383       NaN
14883    mp-1262087    (0, 1, 0)     1   Al4Bi12O36      8090         HO2           4.863797  1.438414
>>> adE_OOH.loc[12100]
bulk_id             mp-1262087
miller_index         (0, 1, 0)
nads                         1
bulk_symbols        Al4Bi12O36
slab_sid                  8090
ads_symbols                HO2
adsorption_energy     3.425383
Name: 12100, dtype: object
>>> adE_OOH.loc[14883]
bulk_id             mp-1262087
miller_index         (0, 1, 0)
nads                         1
bulk_symbols        Al4Bi12O36
slab_sid                  8090
ads_symbols                HO2
adsorption_energy     4.863797
Name: 14883, dtype: object
>>> 4.863797 - 3.425383
1.4384139999999999
```

```
>>> OOH_duplicates3
           bulk_id miller_index  nads bulk_symbols  slab_sid ads_symbols  adsorption_energy      diff
system_id
9845      mp-867583    (1, 0, 0)     1  Ag12Sb12O36     23159         HO2           3.502016       NaN
33068     mp-867583    (1, 0, 0)     1  Ag12Sb12O36     30006         HO2           4.683349  1.181334
>>> adE.loc[9845]
bulk_id              mp-867583
miller_index         (1, 0, 0)
nads                         1
bulk_symbols       Ag12Sb12O36
slab_sid                 23159
ads_symbols                HO2
adsorption_energy     3.502016
Name: 9845, dtype: object
>>> adE.loc[33068]
bulk_id              mp-867583
miller_index         (1, 0, 0)
nads                         1
bulk_symbols       Ag12Sb12O36
slab_sid                 30006
ads_symbols                HO2
adsorption_energy     4.683349
Name: 33068, dtype: object
>>> 4.683349 - 3.502016
1.181333
```