**initial\_LJ\_sanity\_check230616**

total error sum 0.189379, count 521 (546 forces, 6 energies)

sum of force-errors = 1.855391e-01 ( 97.972% - av: 0.000340)

sum of energy-errors = 3.840373e-03 ( 2.028% )

rms-errors:

force 1.843408e-02 (18.434078 meV/A)

energy 2.529945e-03 (2.529945 meV)

force [meV/A] energy [meV] stress [MPa] error sum

RMS: 1.843408e+01 2.529945e+00 5.448924e-03 0.189379

# global energy weight w is 100.000000

# nr. conf\_w w\*de^2 e e0 |e-e0| e-e0 de/e0

0 1.00 0.000299 -4.3741443917 -4.3758743000 0.001730 0.001730 -0.000395

1 1.00 0.000319 -4.3285067373 -4.3302920000 0.001785 0.001785 -0.000412

2 1.00 0.000327 -4.3146601274 -4.3164690000 0.001809 0.001809 -0.000419

3 1.00 0.000419 -4.1739444877 -4.1759910000 0.002047 0.002047 -0.000490

4 1.00 0.001338 -3.3231673321 -3.3195090000 0.003658 -0.003658 0.001102

5 1.00 0.001138 -3.2705944788 -3.267221000 0.003373 -0.003373 0.001033

**initial\_morse\_fit\_230616**

total error sum 8.115488, count 522 (546 forces, 6 energies)

sum of force-errors = 3.802988e+00 ( 46.861% - av: 0.006965)

sum of energy-errors = 4.312500e+00 ( 53.139% )

rms-errors:

force 8.345766e-02 (83.457656 meV/A)

energy 8.477912e-02 (84.779123 meV)

force [meV/A] energy [meV] stress [MPa] error sum

RMS: 8.345766e+01 8.477912e+01 6.731614e+01 8.115488

# global energy weight w is 100.000000

# nr. conf\_w w\*de^2 e e0 |e-e0| e-e0 de/e0

0 1.00 0.257879 -4.3250925437 -4.3758743000 0.050782 0.050782 -0.011605

1 1.00 0.274848 -4.2778660675 -4.3302920000 0.052426 0.052426 -0.012107

2 1.00 0.271655 -4.2643484327 -4.3164690000 0.052121 0.052121 -0.012075

3 1.00 0.279794 -4.1230954356 -4.1759910000 0.052896 0.052896 -0.012667

4 1.00 1.673914 -3.4488888178 -3.3195090000 0.129380 -0.129380 0.038976

5 1.00 1.554410 -3.3918969851 -3.2672210000 0.124676 -0.124676 0.038160

**040716\_morse\_fit\_diff\_evo**

total error sum 8.115700, count 522 (546 forces, 6 energies)

sum of force-errors = 3.802995e+00 ( 46.860% - av: 0.006965)

sum of energy-errors = 4.312704e+00 ( 53.140% )

rms-errors:

force 8.345773e-02 (83.457730 meV/A)

energy 8.478113e-02 (84.781133 meV)

force [meV/A] energy [meV] stress [MPa] error sum

RMS: 8.345773e+01 8.478113e+01 1.265892e-01 8.115700

# global energy weight w is 100.000000

# nr. conf\_w w\*de^2 e e0 |e-e0| e-e0 de/e0

0 1.00 0.257982 -4.3250823952 -4.3758743000 0.050792 0.050792 -0.011607

1 1.00 0.274956 -4.2778557618 -4.3302920000 0.052436 0.052436 -0.012109

2 1.00 0.271764 -4.2643380302 -4.3164690000 0.052131 0.052131 -0.012077

3 1.00 0.279917 -4.1230838291 -4.1759910000 0.052907 0.052907 -0.012669

4 1.00 1.673846 -3.4488862140 -3.3195090000 0.129377 -0.129377 0.038975

5 1.00 1.554240 -3.3918901480 -3.2672210000 0.124669 -0.124669 0.038158

**060716\_stress\_sim\_ann\_all**

total error sum 8.115488, count 594 (546 forces, 6 energies, 36 stresses)

sum of force-errors = 3.802988e+00 ( 46.861% - av: 0.006965)

sum of energy-errors = 4.312500e+00 ( 53.139% )

sum of stress-errors = 0.000000e+00 ( 0.000% )

rms-errors:

force 8.345766e-02 (83.457656 meV/A)

energy 8.477912e-02 (84.779123 meV)

stress 0.000000e+00 (0.000000 MPa)

force [meV/A] energy [meV] stress [MPa] error sum

RMS: 8.345766e+01 8.477912e+01 0.000000e+00 8.115488

# global energy weight w is 100.000000

# nr. conf\_w w\*de^2 e e0 |e-e0| e-e0 de/e0

0 1.00 0.257879 -4.3250925437 -4.3758743000 0.050782 0.050782 -0.011605

1 1.00 0.274848 -4.2778660675 -4.3302920000 0.052426 0.052426 -0.012107

2 1.00 0.271655 -4.2643484327 -4.3164690000 0.052121 0.052121 -0.012075

3 1.00 0.279794 -4.1230954356 -4.1759910000 0.052896 0.052896 -0.012667

4 1.00 1.673914 -3.4488888178 -3.3195090000 0.129380 -0.129380 0.038976

5 1.00 1.554410 -3.3918969851 -3.2672210000 0.124676 -0.124676 0.038160