

# Lattice Constants Report

## Lattice Constants MAE Table

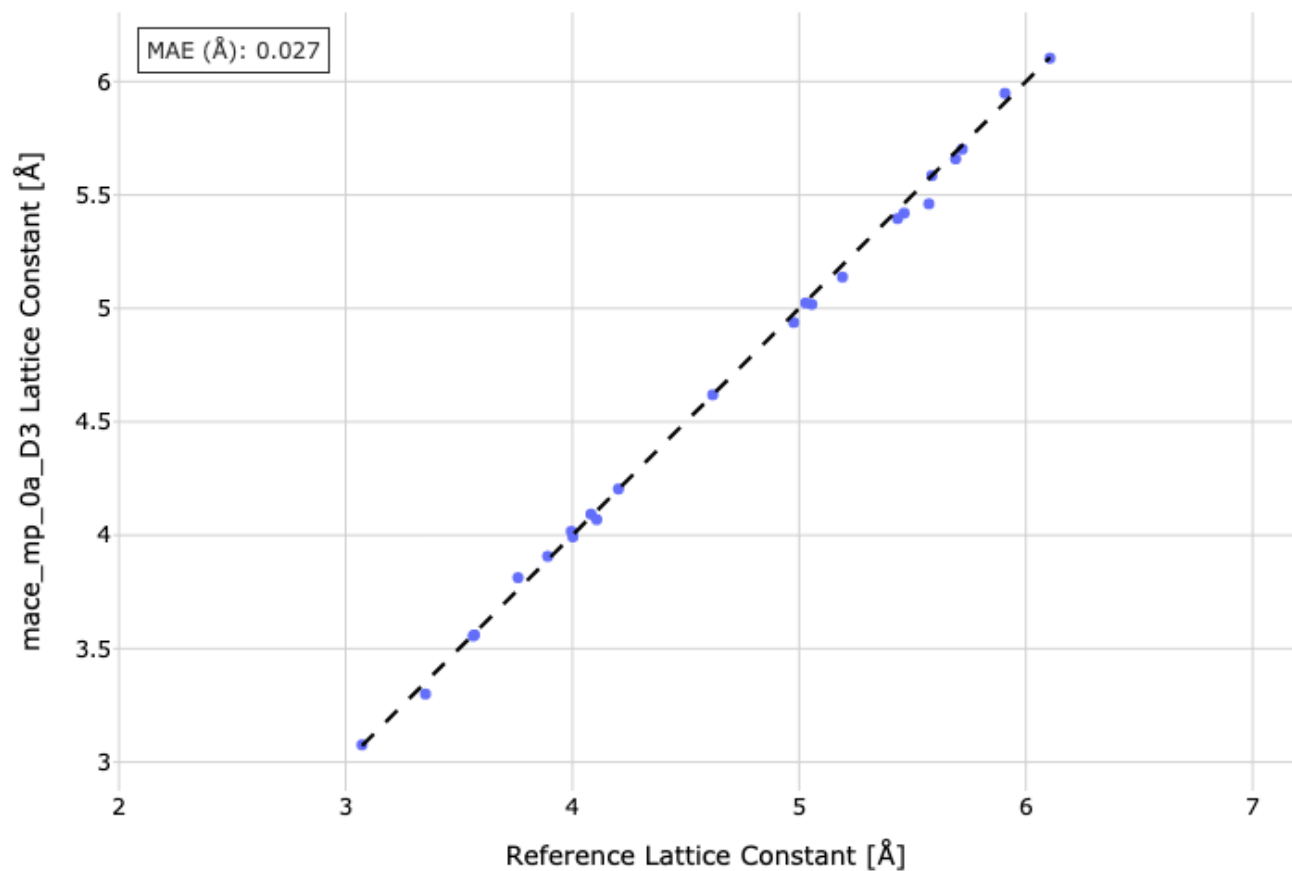
| Model                   | Lat Const [ $\text{\AA}$ ] | Rank |
|-------------------------|----------------------------|------|
| mace_mp_0a_D3           | 0.027                      | 2    |
| mace_mp_0b3_D3          | 0.027                      | 2    |
| mace_mpa_0_D3           | 0.019                      | 1    |
| mace_omat_0_D3          | 0.067                      | 6    |
| mace_matpes_PBE_0_D3    | 0.035                      | 4    |
| mace_matpes_r2scan_0_D3 | 0.044                      | 5    |

## Per-Model Tables and Scatter Plots

mace\_mp\_0a\_D3

| Element | DFT ( $\text{\AA}$ ) | mace_mp_0a_D3 ( $\text{\AA}$ ) | $\Delta$ | $\Delta/\%$ |
|---------|----------------------|--------------------------------|----------|-------------|
| Ag      | 4.082                | 4.093                          | 0.011    | 0.27        |
| Pd      | 3.891                | 3.907                          | 0.016    | 0.41        |
| Rh      | 3.76                 | 3.813                          | 0.053    | 1.41        |
| Li      | 3.352                | 3.3                            | -0.052   | -1.55       |
| Na      | 4.107                | 4.069                          | -0.038   | -0.93       |
| K       | 5.191                | 5.138                          | -0.053   | -1.02       |
| Rb      | 5.572                | 5.461                          | -0.111   | -1.99       |
| Cs      | 6.106                | 6.103                          | -0.003   | -0.05       |
| Ca      | 5.463                | 5.42                           | -0.043   | -0.79       |
| Sr      | 5.908                | 5.948                          | 0.04     | 0.68        |
| Ba      | 4.976                | 4.938                          | -0.038   | -0.76       |
| Al      | 4.002                | 3.993                          | -0.009   | -0.22       |
| LiF     | 3.995                | 4.017                          | 0.022    | 0.55        |
| NaF     | 4.619                | 4.619                          | 0        | 0           |
| NaCl    | 5.585                | 5.585                          | 0        | 0           |
| MgO     | 4.203                | 4.204                          | 0.001    | 0.02        |
| Si      | 5.434                | 5.396                          | -0.038   | -0.7        |
| Ge      | 5.719                | 5.702                          | -0.017   | -0.3        |
| GaAs    | 5.69                 | 5.659                          | -0.031   | -0.54       |
| Cu      | 3.568                | 3.561                          | -0.007   | -0.2        |
| C       | 3.562                | 3.556                          | -0.006   | -0.17       |
| LiCl    | 5.056                | 5.018                          | -0.038   | -0.75       |
| SiC(a)  | 3.072                | 3.076                          | 0.004    | 0.13        |
| SiC(c)  | 5.029                | 5.024                          | -0.005   | -0.1        |

## mace\_mp\_0a\_D3 — Lattice Constant

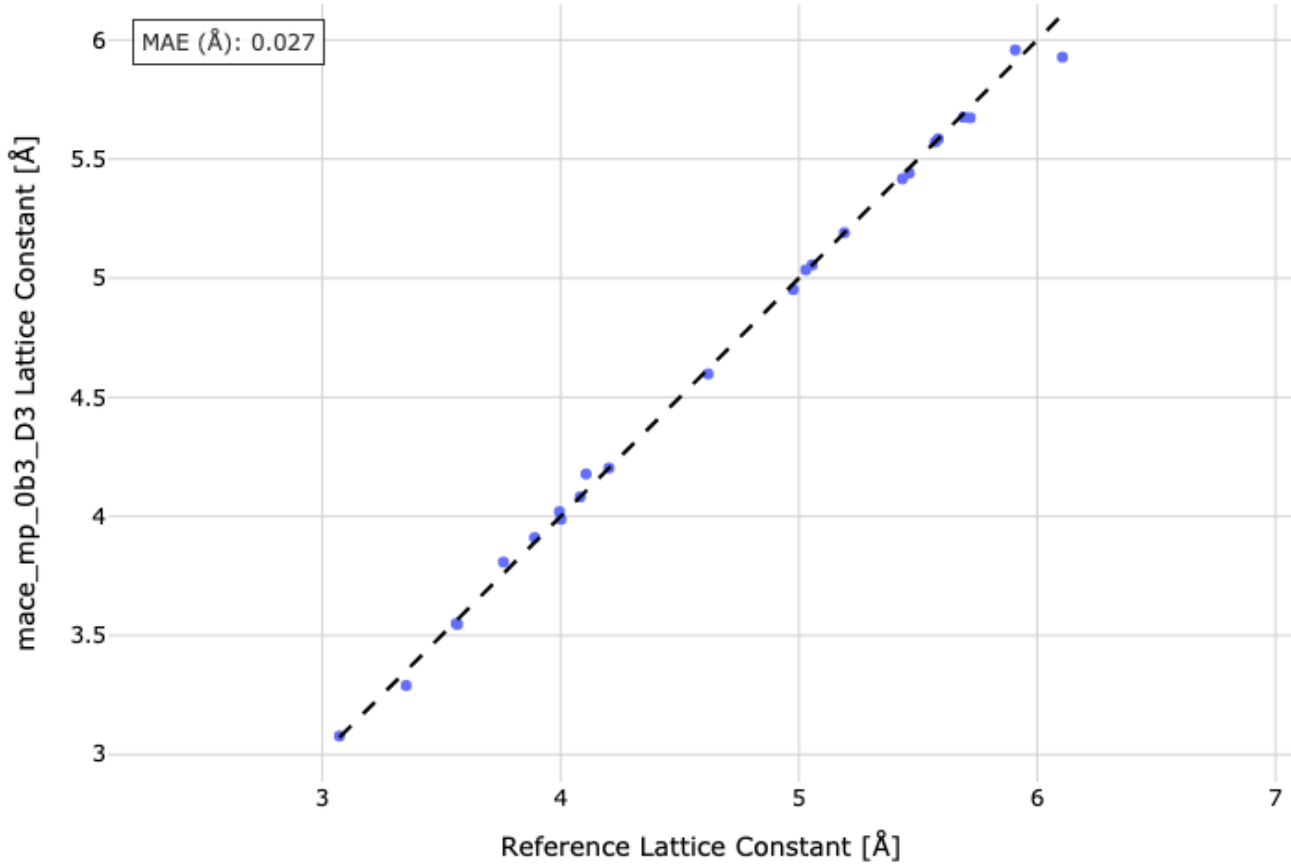


## mace\_mp\_0b3\_D3

| Element | DFT (Å) | mace_mp_0b3_D3 (Å) | $\Delta$ | $\Delta/\%$ |
|---------|---------|--------------------|----------|-------------|
| Ag      | 4.082   | 4.082              | 0        | 0           |
| Pd      | 3.891   | 3.911              | 0.02     | 0.51        |
| Rh      | 3.76    | 3.808              | 0.048    | 1.28        |
| Li      | 3.352   | 3.29               | -0.062   | -1.85       |
| Na      | 4.107   | 4.178              | 0.071    | 1.73        |
| K       | 5.191   | 5.191              | 0        | 0           |
| Rb      | 5.572   | 5.572              | 0        | 0           |
| Cs      | 6.106   | 5.928              | -0.178   | -2.92       |
| Ca      | 5.463   | 5.441              | -0.022   | -0.4        |
| Sr      | 5.908   | 5.958              | 0.05     | 0.85        |
| Ba      | 4.976   | 4.952              | -0.024   | -0.48       |
| Al      | 4.002   | 3.988              | -0.014   | -0.35       |
| LiF     | 3.995   | 4.02               | 0.025    | 0.63        |
| NaF     | 4.619   | 4.598              | -0.021   | -0.45       |
| NaCl    | 5.585   | 5.585              | 0        | 0           |
| MgO     | 4.203   | 4.203              | 0        | 0           |
| Si      | 5.434   | 5.417              | -0.017   | -0.31       |
| Ge      | 5.719   | 5.673              | -0.046   | -0.8        |

| Element | DFT ( $\text{\AA}$ ) | mace_mp_0b3_D3 ( $\text{\AA}$ ) | $\Delta$ | $\Delta/\%$ |
|---------|----------------------|---------------------------------|----------|-------------|
| GaAs    | 5.69                 | 5.676                           | -0.014   | -0.25       |
| Cu      | 3.568                | 3.547                           | -0.021   | -0.59       |
| C       | 3.562                | 3.55                            | -0.012   | -0.34       |
| LiCl    | 5.056                | 5.056                           | 0        | 0           |
| SiC(a)  | 3.072                | 3.078                           | 0.006    | 0.2         |
| SiC(c)  | 5.029                | 5.035                           | 0.006    | 0.12        |

### mace\_mp\_0b3\_D3 — Lattice Constant

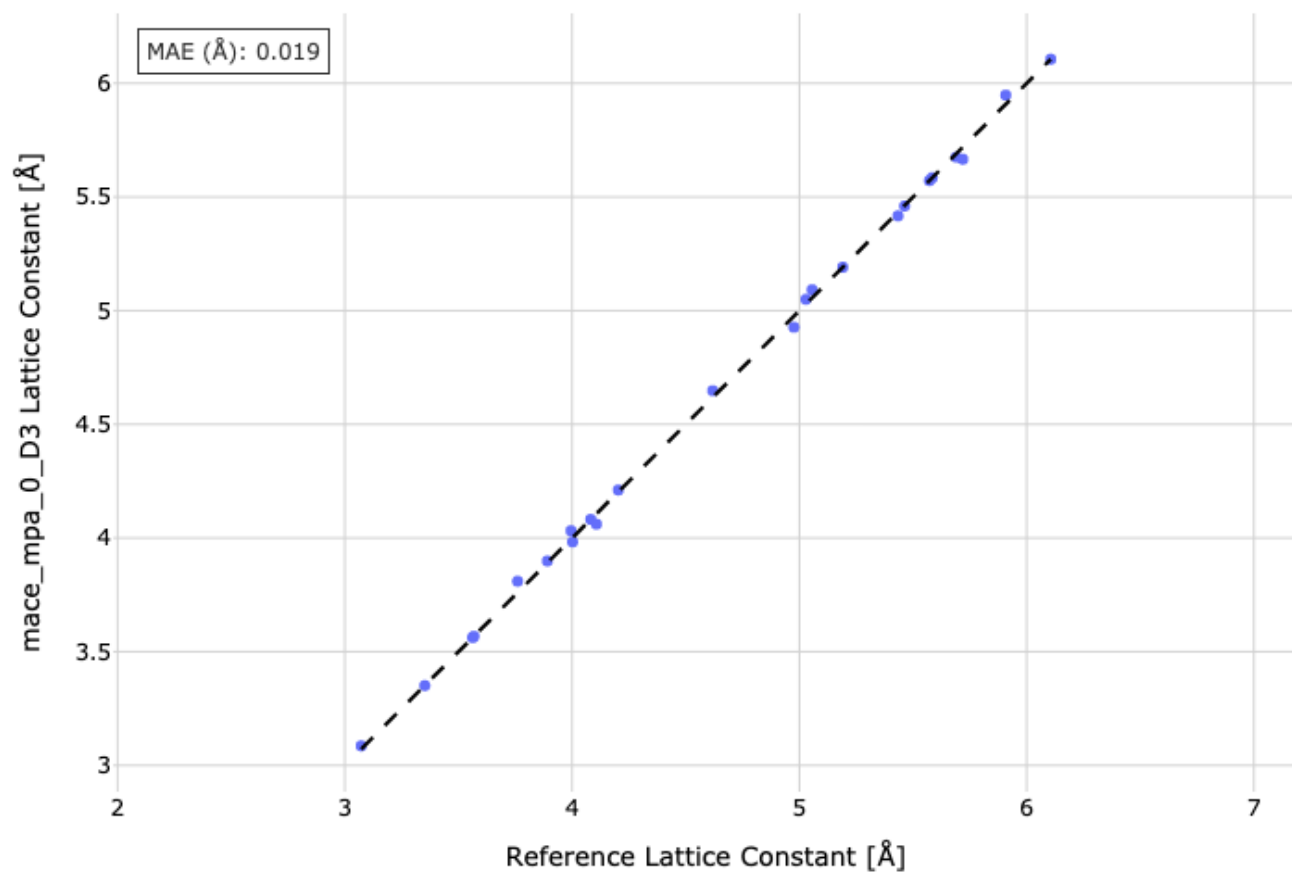


### mace\_mpa\_0\_D3

| Element | DFT ( $\text{\AA}$ ) | mace_mpa_0_D3 ( $\text{\AA}$ ) | $\Delta$ | $\Delta/\%$ |
|---------|----------------------|--------------------------------|----------|-------------|
| Ag      | 4.082                | 4.082                          | 0        | 0           |
| Pd      | 3.891                | 3.899                          | 0.008    | 0.21        |
| Rh      | 3.76                 | 3.81                           | 0.05     | 1.33        |
| Li      | 3.352                | 3.351                          | -0.001   | -0.03       |
| Na      | 4.107                | 4.061                          | -0.046   | -1.12       |
| K       | 5.191                | 5.191                          | 0        | 0           |
| Rb      | 5.572                | 5.572                          | 0        | 0           |
| Cs      | 6.106                | 6.106                          | 0        | 0           |

| Element | DFT ( $\text{\AA}$ ) | mace_mpa_0_D3 ( $\text{\AA}$ ) | $\Delta$ | $\Delta/\%$ |
|---------|----------------------|--------------------------------|----------|-------------|
| Ca      | 5.463                | 5.46                           | -0.003   | -0.05       |
| Sr      | 5.908                | 5.948                          | 0.04     | 0.68        |
| Ba      | 4.976                | 4.927                          | -0.049   | -0.98       |
| Al      | 4.002                | 3.983                          | -0.019   | -0.47       |
| LiF     | 3.995                | 4.032                          | 0.037    | 0.93        |
| NaF     | 4.619                | 4.648                          | 0.029    | 0.63        |
| NaCl    | 5.585                | 5.585                          | 0        | 0           |
| MgO     | 4.203                | 4.211                          | 0.008    | 0.19        |
| Si      | 5.434                | 5.417                          | -0.017   | -0.31       |
| Ge      | 5.719                | 5.666                          | -0.053   | -0.93       |
| GaAs    | 5.69                 | 5.675                          | -0.015   | -0.26       |
| Cu      | 3.568                | 3.568                          | 0        | 0           |
| C       | 3.562                | 3.562                          | 0        | 0           |
| LiCl    | 5.056                | 5.092                          | 0.036    | 0.71        |
| SiC(a)  | 3.072                | 3.086                          | 0.014    | 0.46        |
| SiC(c)  | 5.029                | 5.05                           | 0.021    | 0.42        |

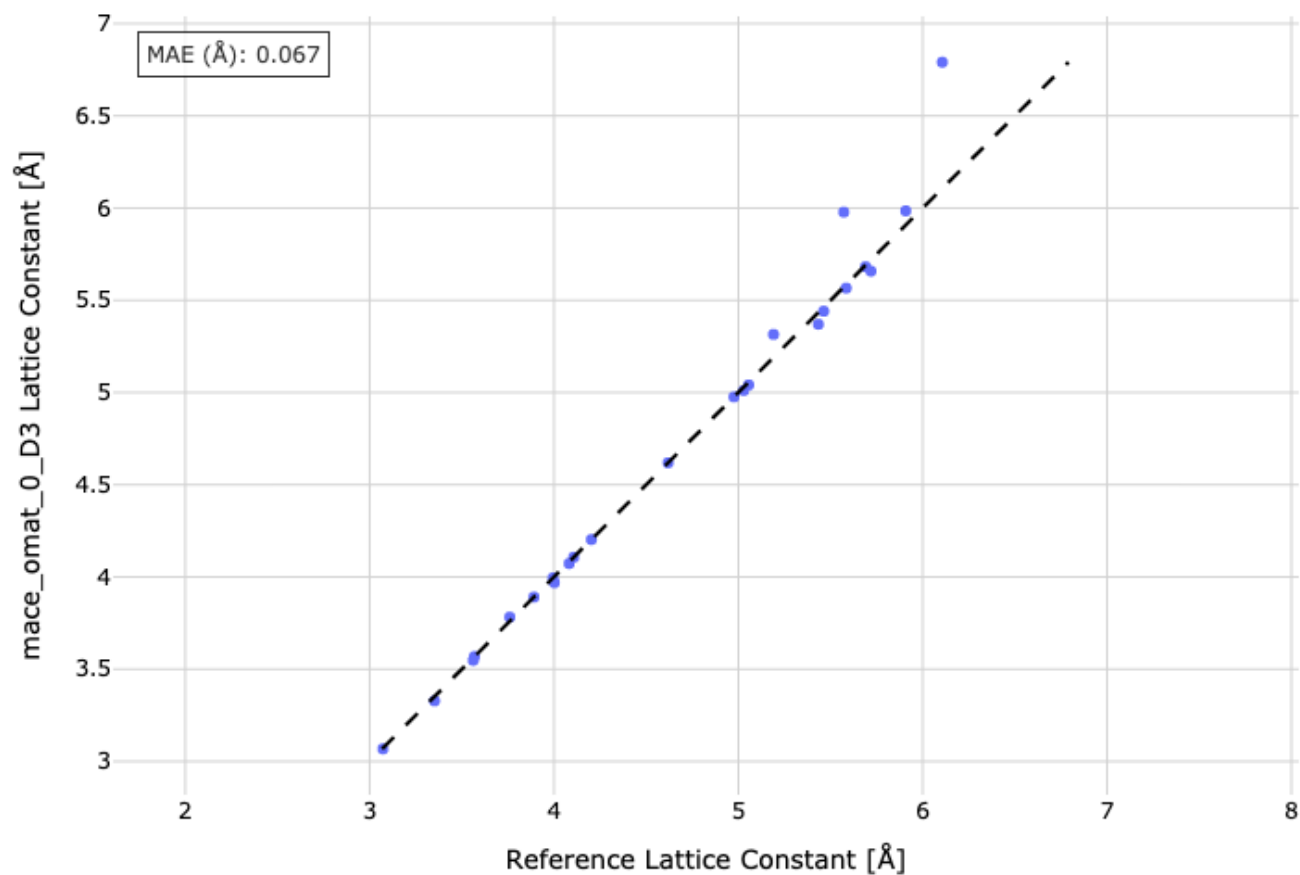
mace\_mpa\_0\_D3 — Lattice Constant



mace\_omat\_0\_D3

| Element | DFT (Å) | mace_omat_0_D3 (Å) | $\Delta$ | $\Delta/\%$ |
|---------|---------|--------------------|----------|-------------|
| Ag      | 4.082   | 4.073              | -0.009   | -0.22       |
| Pd      | 3.891   | 3.891              | 0        | 0           |
| Rh      | 3.76    | 3.782              | 0.022    | 0.59        |
| Li      | 3.352   | 3.328              | -0.024   | -0.72       |
| Na      | 4.107   | 4.107              | 0        | 0           |
| K       | 5.191   | 5.315              | 0.124    | 2.39        |
| Rb      | 5.572   | 5.978              | 0.406    | 7.29        |
| Cs      | 6.106   | 6.791              | 0.685    | 11.22       |
| Ca      | 5.463   | 5.441              | -0.022   | -0.4        |
| Sr      | 5.908   | 5.985              | 0.077    | 1.3         |
| Ba      | 4.976   | 4.976              | 0        | 0           |
| Al      | 4.002   | 3.969              | -0.033   | -0.82       |
| LiF     | 3.995   | 3.995              | 0        | 0           |
| NaF     | 4.619   | 4.619              | 0        | 0           |
| NaCl    | 5.585   | 5.566              | -0.019   | -0.34       |
| MgO     | 4.203   | 4.203              | 0        | 0           |
| Si      | 5.434   | 5.37               | -0.064   | -1.18       |
| Ge      | 5.719   | 5.658              | -0.061   | -1.07       |
| GaAs    | 5.69    | 5.682              | -0.008   | -0.14       |
| Cu      | 3.568   | 3.568              | 0        | 0           |
| C       | 3.562   | 3.548              | -0.014   | -0.39       |
| LiCl    | 5.056   | 5.041              | -0.015   | -0.3        |
| SiC(a)  | 3.072   | 3.068              | -0.004   | -0.13       |
| SiC(c)  | 5.029   | 5.011              | -0.018   | -0.36       |

## mace\_omat\_0\_D3 — Lattice Constant

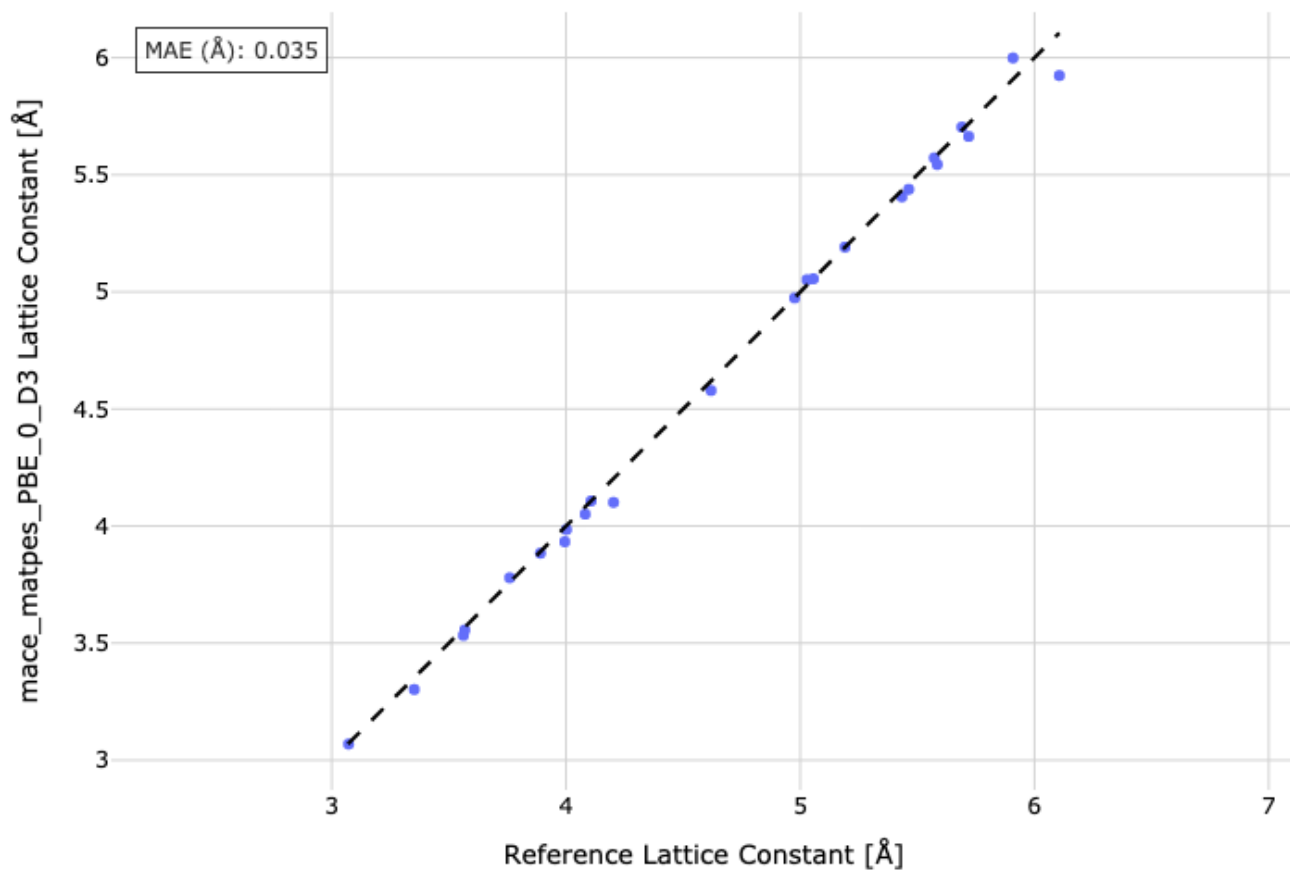


## mace\_matpes\_PBE\_0\_D3

| Element | DFT (Å) | mace_matpes_PBE_0_D3 (Å) | $\Delta$ | $\Delta/\%$ |
|---------|---------|--------------------------|----------|-------------|
| Ag      | 4.082   | 4.051                    | -0.031   | -0.76       |
| Pd      | 3.891   | 3.884                    | -0.007   | -0.18       |
| Rh      | 3.76    | 3.779                    | 0.019    | 0.51        |
| Li      | 3.352   | 3.302                    | -0.05    | -1.49       |
| Na      | 4.107   | 4.107                    | 0        | 0           |
| K       | 5.191   | 5.191                    | 0        | 0           |
| Rb      | 5.572   | 5.572                    | 0        | 0           |
| Cs      | 6.106   | 5.924                    | -0.182   | -2.98       |
| Ca      | 5.463   | 5.438                    | -0.025   | -0.46       |
| Sr      | 5.908   | 5.999                    | 0.091    | 1.54        |
| Ba      | 4.976   | 4.974                    | -0.002   | -0.04       |
| Al      | 4.002   | 3.985                    | -0.017   | -0.42       |
| LiF     | 3.995   | 3.933                    | -0.062   | -1.55       |
| NaF     | 4.619   | 4.579                    | -0.04    | -0.87       |
| NaCl    | 5.585   | 5.544                    | -0.041   | -0.73       |
| MgO     | 4.203   | 4.101                    | -0.102   | -2.43       |
| Si      | 5.434   | 5.406                    | -0.028   | -0.52       |
| Ge      | 5.719   | 5.664                    | -0.055   | -0.96       |

| Element | DFT ( $\text{\AA}$ ) | mace_matpes_PBE_0_D3 ( $\text{\AA}$ ) | $\Delta$ | $\Delta/\%$ |
|---------|----------------------|---------------------------------------|----------|-------------|
| GaAs    | 5.69                 | 5.704                                 | 0.014    | 0.25        |
| Cu      | 3.568                | 3.556                                 | -0.012   | -0.34       |
| C       | 3.562                | 3.533                                 | -0.029   | -0.81       |
| LiCl    | 5.056                | 5.056                                 | 0        | 0           |
| SiC(a)  | 3.072                | 3.069                                 | -0.003   | -0.1        |
| SiC(c)  | 5.029                | 5.052                                 | 0.023    | 0.46        |

mace\_matpes\_PBE\_0\_D3 — Lattice Constant



mace\_matpes\_r2scan\_0\_D3

| Element | DFT ( $\text{\AA}$ ) | mace_matpes_r2scan_0_D3 ( $\text{\AA}$ ) | $\Delta$ | $\Delta/\%$ |
|---------|----------------------|------------------------------------------|----------|-------------|
| Ag      | 4.082                | 4.067                                    | -0.015   | -0.37       |
| Pd      | 3.891                | 3.895                                    | 0.004    | 0.1         |
| Rh      | 3.76                 | 3.812                                    | 0.052    | 1.38        |
| Li      | 3.352                | 3.373                                    | 0.021    | 0.63        |
| Na      | 4.107                | 4.107                                    | 0        | 0           |
| K       | 5.191                | 5.248                                    | 0.057    | 1.1         |
| Rb      | 5.572                | 5.572                                    | 0        | 0           |
| Cs      | 6.106                | 6.053                                    | -0.053   | -0.87       |

| Element | DFT ( $\text{\AA}$ ) | mace_matpes_r2scan_0_D3 ( $\text{\AA}$ ) | $\Delta$ | $\Delta/\%$ |
|---------|----------------------|------------------------------------------|----------|-------------|
| Ca      | 5.463                | 5.557                                    | 0.094    | 1.72        |
| Sr      | 5.908                | 6.096                                    | 0.188    | 3.18        |
| Ba      | 4.976                | 4.976                                    | 0        | 0           |
| Al      | 4.002                | 3.963                                    | -0.039   | -0.97       |
| LiF     | 3.995                | 3.925                                    | -0.07    | -1.75       |
| NaF     | 4.619                | 4.522                                    | -0.097   | -2.1        |
| NaCl    | 5.585                | 5.479                                    | -0.106   | -1.9        |
| MgO     | 4.203                | 4.164                                    | -0.039   | -0.93       |
| Si      | 5.434                | 5.415                                    | -0.019   | -0.35       |
| Ge      | 5.719                | 5.622                                    | -0.097   | -1.7        |
| GaAs    | 5.69                 | 5.671                                    | -0.019   | -0.33       |
| Cu      | 3.568                | 3.547                                    | -0.021   | -0.59       |
| C       | 3.562                | 3.575                                    | 0.013    | 0.36        |
| LiCl    | 5.056                | 5.017                                    | -0.039   | -0.77       |
| SiC(a)  | 3.072                | 3.074                                    | 0.002    | 0.07        |
| SiC(c)  | 5.029                | 5.047                                    | 0.018    | 0.36        |

mace\_matpes\_r2scan\_0\_D3 — Lattice Constant

