# Model weights and average features of in-domain tests

The mean absolute model weights, $c$, with respect to the features corresponding to each body-order $K$ are tabulated in Table 1 and 2 for the purified and self-interacting bases, respectively. These results verify that potentials with purified bases have negligible coefficients for features $K$ that have orders higher than the maximum number of atoms in the structures of the training set. Potentials with the original ACE bases will have higher order $K$ features that are relevant due to the spurious self-interactions masked as lower-order terms. The peculiar case of the $Si_2$-trained potentials stem from the fact that the $K = 2$ functions used (24 functions in the chosen basis) are already sufficient in capturing the pair interactions of the training set which only contains dimers. This applies to both purified and self-interacting bases, making the self-interacting basis functions practically unnecessary in capturing the correct two-body energetics.

Table 1: Mean absolute model weights for the features each $K$ of the in-domain tests for the purified bases

| Trainset | Basis | Feature | | | |
|---|---|---|---|---|---|
| | | $K = 2$ | $K = 3$ | $K = 4$ | $K = 5$ |
| $Si_2$ | 24.20 | 2.024 | $< 10^{-8}$ | | |
| | 24.20.16 | 2.024 | $< 10^{-8}$ | $< 10^{-8}$ | |
| | 24.20.16.12 | 2.024 | $< 10^{-8}$ | $< 10^{-8}$ | $< 10^{-8}$ |
| $Si_{23}$ | 24.20 | 1.85 | 0.392 | | |
| | 24.20.16 | 1.85 | 0.392 | $< 10^{-8}$ | |
| | 24.20.16.12 | 1.85 | 0.392 | $< 10^{-8}$ | $< 10^{-8}$ |
| $Si_{234}$ | 24.20 | 1.569 | 0.421 | | |
| | 24.20.16 | 1.716 | 0.296 | 0.495 | |
| | 24.20.16.12 | 1.716 | 0.296 | 0.495 | $< 10^{-8}$ |
| $Si_{2345}$ | 24.20 | 1.429 | 0.315 | | |
| | 24.20.16 | 1.420 | 0.291 | 0.434 | |
| | 24.20.16.12 | 1.370 | 0.314 | 0.482 | 0.574 |

Table 2: Mean absolute model weights for the features each $K$ of the in-domain tests for the self-interacting bases

| Trainset | Basis | Feature | | | |
|---|---|---|---|---|---|
| | | $K = 2$ | $K = 3$ | $K = 4$ | $K = 5$ |
| $Si_2$ | 24.20 | 2.024 | $< 10^{-8}$ | | |
| | 24.20.16 | 2.024 | $< 10^{-8}$ | $< 10^{-8}$ | |
| | 24.20.16.12 | 2.024 | $< 10^{-8}$ | $< 10^{-8}$ | $< 10^{-8}$ |
| $Si_{23}$ | 24.20 | 1.85 | 0.392 | | |
| | 24.20.16 | 1.84 | 0.330 | 0.146 | |
| | 24.20.16.12 | 1.85 | 0.329 | 0.142 | 0.0779 |
| $Si_{234}$ | 24.20 | 1.569 | 0.421 | | |
| | 24.20.16 | 1.714 | 0.359 | 0.485 | |
| | 24.20.16.12 | 1.708 | 0.333 | 0.431 | 0.315 |
| $Si_{2345}$ | 24.20 | 1.429 | 0.315 | | |
| | 24.20.16 | 1.410 | 0.280 | 0.372 | |
| | 24.20.16.12 | 1.355 | 0.371 | 0.497 | 0.521 |