**Table 1.** Lennard-Jones parameters of framework atoms.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Type** | **(ε/kB)[K]** | **σ[Å]** | **Type** | **(ε/kB)[K]** | **σ[Å]** | **Type** | **(ε/kB)[K]** | **σ[Å]** |
| H\_ | 22.1565 | 2.5711 | Br\_ | 126.392 | 3.732 | Yb\_ | 114.81 | 2.989 |
| D\_ | 22.1565 | 2.5711 | Kr\_ | 110.782 | 3.6892 | Lu\_ | 20.6458 | 3.2429 |
| He\_ | 28.1991 | 2.1043 | Rb\_ | 20.1422 | 3.6652 | Hf\_ | 36.256 | 2.7983 |
| Li\_ | 12.5889 | 2.1836 | Sr\_ | 118.335 | 3.2438 | Ta\_ | 40.788 | 2.8241 |
| Be\_ | 42.8022 | 2.4455 | Y\_ | 36.256 | 2.9801 | W\_ | 33.7382 | 2.7342 |
| B\_ | 90.64 | 3.6375 | Zr\_ | 34.7453 | 2.7832 | Re\_ | 33.2347 | 2.6317 |
| C\_ | 52.8734 | 3.4309 | Nb\_ | 29.7098 | 2.8197 | Os\_ | 18.6316 | 2.7796 |
| N\_ | 34.7453 | 3.2607 | Mo\_ | 28.1991 | 2.719 | Ir\_ | 36.7596 | 2.5302 |
| O\_ | 30.2133 | 3.1181 | Tc\_ | 24.1707 | 2.6709 | Pt\_ | 40.2845 | 2.4535 |
| F\_ | 25.1778 | 2.997 | Ru\_ | 28.1991 | 2.6397 | Au\_ | 19.6387 | 2.9337 |
| Ne\_ | 21.1493 | 2.8892 | Rh\_ | 26.6885 | 2.6094 | Hg\_ | 193.869 | 2.4099 |
| Na\_ | 15.1067 | 2.6576 | Pd\_ | 24.1707 | 2.5827 | Tl\_ | 342.417 | 3.8727 |
| Mg\_ | 55.8947 | 2.6914 | Ag\_ | 18.128 | 2.8045 | Pb\_ | 333.857 | 3.8282 |
| Al\_ | 254.295 | 4.0082 | Cd\_ | 114.81 | 2.5373 | Bi\_ | 260.841 | 3.8932 |
| Si\_ | 202.429 | 3.8264 | In\_ | 301.629 | 3.9761 | Po\_ | 163.655 | 4.1952 |
| P\_ | 153.584 | 3.6946 | Sn\_ | 285.516 | 3.9128 | At\_ | 143.009 | 4.2318 |
| S\_ | 137.974 | 3.5948 | Sb\_ | 226.096 | 3.9378 | Rn\_ | 124.881 | 4.2451 |
| Cl\_ | 114.307 | 3.5164 | Te\_ | 200.415 | 3.9823 | Fr\_ | 25.1778 | 4.3654 |
| Ar\_ | 93.1578 | 3.446 | I\_ | 170.705 | 4.009 | Ra\_ | 203.436 | 3.2758 |
| K\_ | 17.6245 | 3.3961 | Xe\_ | 167.18 | 3.9235 | Ac\_ | 16.6173 | 3.0985 |
| Ca\_ | 119.846 | 3.0282 | Cs\_ | 22.66 | 4.0242 | Th\_ | 13.0925 | 3.0255 |
| Sc\_ | 9.5676 | 2.9355 | Ba\_ | 183.294 | 3.299 | Pa\_ | 11.0782 | 3.0504 |
| Ti\_ | 8.5604 | 2.8286 | La\_ | 8.5604 | 3.1377 | U\_ | 11.0782 | 3.0246 |
| V\_ | 8.0569 | 2.801 | Ce\_ | 6.5462 | 3.168 | Np\_ | 9.5676 | 3.0504 |
| Cr\_ | 7.5533 | 2.6932 | Pr\_ | 5.0356 | 3.2126 | Pu\_ | 8.0569 | 3.0504 |
| Mn\_ | 6.5462 | 2.638 | Nd\_ | 5.0356 | 3.185 | Am\_ | 7.0498 | 3.0121 |
| Fe\_ | 6.5462 | 2.5943 | Pm\_ | 4.532 | 3.16 | Cm\_ | 6.5462 | 2.9631 |
| Co\_ | 7.0498 | 2.5587 | Sm\_ | 4.0284 | 3.136 | Bk\_ | 6.5462 | 2.9747 |
| Ni\_ | 7.5533 | 2.5248 | Eu\_ | 4.0284 | 3.1119 | Cf\_ | 6.5462 | 2.9515 |
| Cu\_ | 2.5178 | 3.1137 | Gd\_ | 4.532 | 3.0005 | Es\_ | 6.0427 | 2.9391 |
| Zn\_ | 62.4409 | 2.4616 | Tb\_ | 3.5249 | 3.0745 | Fm\_ | 6.0427 | 2.9275 |
| Ga\_ | 208.975 | 3.9048 | Dy\_ | 3.5249 | 3.054 | Md\_ | 5.5391 | 2.9168 |
| **Type** | **(ε/kB)[K]** | **σ[Å]** | **Type** | **(ε/kB)[K]** | **σ[Å]** | **Type** | **(ε/kB)[K]** | **σ[Å]** |
| Ge\_ | 190.847 | 3.813 | Ho\_ | 3.5249 | 3.0371 | No\_ | 5.5391 | 2.8936 |
| As\_ | 155.598 | 3.7685 | Er\_ | 3.5249 | 3.021 | Lw\_ | 5.5391 | 2.8829 |
| Se\_ | 146.534 | 3.7462 | Tm\_ | 3.0213 | 3.0059 | He | 10.9 | 2.64 |
| CH4\_sp3 | 148 | 3.73 | H2\_unit | 34.2 | 2.96 | O\_co2 | 79 | 3.05 |
| C\_co2 | 27 | 2.8 | N\_n2 | 36.4 | 3.32 | N\_com | none |  |
| Ow | 77.94 | 3.15365 | O\_o2 | 49.0 | 3.020 | O\_com | none |  |