# Vdb/CASTEP

Legacy Vanderbilt-type USPP dataset/ CASTEP 8.0

`name and version of the code:` CASTEP 8.0
`type of basis set:` plane waves
`method:` ultrasoft pseudopotentials (Legacy Vanderbilt-type Materials Studio set)

## GENERAL INFORMATION

| | |
|---|---|
| `exchange-correlation functional` | PBE |
| `relativistic scheme` | core scalar relativistic (Koelling-Harmon) |
| `assignment of core / valence states` | see table |
| `basis set size` | cutoff energy = 700 eV |
| `k-mesh density` | see table for grid values and number of k-points in the irreducible wedge of the 1st Brillouin zone (# $k$); this choice achieves spacing $\Delta k < 0.125\,\text{Å}^{-1}$ |
| `reciprocal-space integration method` | Gaussian smearing with a fictitious temperature corresponding to 0.2 eV |

## METHOD-SPECIFIC INFORMATION

| | |
|---|---|
| `size of FFT grid for augmentation` | 1.5 × FFT grid for soft density ($E_{c,\rho} = 9\,E_{c,\phi}$) |

## ADDITIONAL COMMENTS

This is the set of pseudopotentials generated using the Vanderbilt USPP code and shipped with Accelrys Materials Studio in ".usp" file format. The ".uspcc" variants incorporating a non-linear core correction were used for Mn, Fe, Co, Ni, Y and Hf.

## REFERENCES


`pseudopotential method`

[1] D. Vanderbilt, *Phys. Rev. B* **41**(11), 7892–7895 (1990).

`code`

[2] S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. I. J. Probert, K. Refson and M. C. Payne, *Z. Kristall.*, **220**, 567–570 (2005).

`scalar relativity`

[3] D. D. Koelling and B. N. Harmon, *J. Phys. C: Solid State* **10**, 3107–3114 (1977).

**Table I.** Calculation settings and results per element: valence, Monkhorst-Pack k-point mesh in the full 1st Brillouin zone of the conventional cell *kpts* and number of irreducible k-points # $k$, equilibrium volume per atom $V_0$, bulk modulus $B_0$, pressure derivative of the bulk modulus $B_1$.

| | Valence | *kpts* | # $k$ | $V_0$ [Å$^3$/atom] | $B_0$ [GPa] | $B_1$ [–] |
|---|---|---|---|---|---|---|
| H | $1s^1$ | 15×15×10 | 135 | 17.563 | 10.447 | 2.825 |
| He | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Li | $1s^2\ 2s^1$ | 19×19×3 | 110 | 20.378 | 13.607 | 3.298 |
| Be | $2s^2$ | 26×26×14 | 1 274 | 7.815 | 119.510 | 2.525 |
| B | $2s^2\ 2p^1$ | 13×13×12 | 546 | 7.191 | 236.678 | 3.444 |
| C | $2s^2\ 2p^2$ | 23×23×6 | 168 | 11.566 | 208.966 | 3.616 |
| N | $2s^2\ 2p^3$ | 8×8×8 | 24 | 33.276 | 52.266 | 3.468 |
| O | $2s^2\ 2p^4$ | 13×12×12 | 468 | 19.380 | 53.250 | 4.455 |
| F | $2s^2\ 2p^5$ | 9×14×8 | 252 | 19.476 | 35.208 | 4.223 |
| Ne | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Na | $2s^2\ 2p^6\ 3s^1$ | 16×16×2 | 136 | 37.271 | 7.664 | 3.790 |
| Mg | $2p^6\ 3s^2$ | 18×18×10 | 450 | 23.264 | 36.071 | 2.214 |
| Al | $3s^2\ 3p^1$ | 13×13×13 | 84 | 16.593 | 76.526 | 4.570 |
| Si | $3s^2\ 3p^2$ | 16×16×16 | 408 | 20.360 | 89.087 | 4.307 |
| P | $3s^2\ 3p^3$ | 15×5×11 | 144 | 20.863 | 70.212 | 4.377 |
| S | $3s^2\ 3p^4$ | 20×20×20 | 770 | 17.077 | 83.151 | 4.114 |
| Cl | $3s^2\ 3p^5$ | 7×12×6 | 72 | 37.283 | 19.795 | 4.379 |
| Ar | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| K | $3s^2\ 3p^6\ 4s^1$ | 10×10×10 | 35 | 73.543 | 3.563 | 3.740 |
| Ca | $3s^2\ 3p^6\ 4s^2$ | 9×9×9 | 35 | 42.230 | 17.102 | 3.063 |
| Sc | $3s^2\ 3p^6\ 3d^1\ 4s^2$ | 18×18×10 | 450 | 24.690 | 53.909 | 3.353 |
| Ti | $3s^2\ 3p^6\ 3d^2\ 4s^2$ | 20×20×11 | 660 | 17.412 | 111.565 | 3.567 |
| V | $3s^2\ 3p^6\ 3d^3\ 4s^2$ | 17×17×17 | 165 | 13.496 | 180.666 | 3.766 |
| Cr | $3s^2\ 3p^6\ 3d^5\ 4s^1$ | 18×18×18 | 165 | 12.460 | 115.824 | 6.232 |
| Mn | $3d^5\ 4s^2$ | 14×14×14 | 196 | 12.081 | 123.543 | 2.491 |
| Fe | $3d^6\ 4s^2$ | 18×18×18 | 165 | 11.137 | 212.468 | 6.366 |
| Co | $3d^7\ 4s^2$ | 23×23×13 | 392 | 11.126 | 213.989 | 5.335 |
| Ni | $3d^8\ 4s^2$ | 14×14×14 | 84 | 11.059 | 199.256 | 4.892 |
| Cu | $3d^{10}\ 4s^1$ | 14×14×14 | 84 | 11.960 | 136.416 | 4.664 |
| Zn | $3d^{10}\ 4s^2$ | 22×22×10 | 660 | 15.008 | 84.946 | 8.260 |
| Ga | $3d^{10}\ 4s^2\ 4p^1$ | 11×7×11 | 144 | 20.422 | 49.593 | 3.104 |
| Ge | $4s^2\ 4p^2$ | 15×15×15 | 120 | 23.622 | 59.973 | 4.862 |
| As | $4s^2\ 4p^3$ | 15×15×5 | 119 | 22.052 | 69.324 | 4.079 |
| Se | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Br | $4s^2\ 4p^5$ | 6×12×6 | 54 | 39.382 | 22.469 | 5.070 |
| Kr | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Rb | $4s^2\ 4p^6\ 5s^1$ | 9×9×9 | 35 | 90.941 | 2.770 | 3.725 |
| Sr | $4s^2\ 4p^6\ 5s^2$ | 9×9×9 | 35 | 55.032 | 11.716 | 3.210 |
| Y | $4d^1\ 5s^2$ | 16×16×9 | 360 | 33.510 | 45.091 | 3.535 |
| Zr | $4s^2\ 4p^6\ 4d^2\ 5s^2$ | 18×18×10 | 450 | 23.367 | 93.570 | 3.328 |
| Nb | $4s^2\ 4p^6\ 4d^4\ 5s^1$ | 15×15×15 | 120 | 18.105 | 169.515 | 3.937 |
| Mo | $4s^2\ 4p^6\ 4d^5\ 5s^1$ | 16×16×16 | 120 | 15.723 | 261.577 | 4.493 |
| Tc | $4s^2\ 4p^6\ 4d^6\ 5s^1$ | 21×21×12 | 288 | 14.392 | 299.655 | 4.523 |
| Ru | $4s^2\ 4p^6\ 4d^7\ 5s^1$ | 21×21×12 | 288 | 13.718 | 313.866 | 4.864 |
| Rh | $4d^8\ 5s^1$ | 13×13×13 | 84 | 14.750 | 249.801 | 5.461 |
| Pd | $4d^{10}$ | 13×13×13 | 84 | 15.164 | 180.989 | 5.761 |
| Ag | $4d^{10}\ 5s^1$ | 12×12×12 | 56 | 17.717 | 97.783 | 5.874 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Cd | $4d^{10}\ 5s^2$ | 19×19×9 | 200 | 23.199 | 42.139 | 7.700 |
| In | $4d^{10}\ 5s^2\ 5p^1$ | 15×15×10 | 180 | 27.671 | 35.185 | 5.254 |
| Sn | $5s^2\ 5p^2$ | 13×13×13 | 84 | 36.862 | 35.402 | 4.373 |
| Sb | $5s^2\ 5p^3$ | 13×13×5 | 91 | 31.072 | 52.528 | 6.939 |
| Te | $5s^2\ 5p^4$ | 13×13×9 | 161 | 35.028 | 45.132 | 5.036 |
| I | $5s^2\ 5p^5$ | 6×11×5 | 54 | 50.510 | 18.649 | 5.215 |
| Xe | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Cs | $5s^2\ 5p^6\ 6s^1$ | 8×8×8 | 20 | 116.710 | 2.086 | −0.828 |
| Ba | $5s^2\ 5p^6\ 6s^2$ | 10×10×10 | 35 | 63.361 | 8.825 | 3.494 |
| Lu | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Hf | $5d^2\ 6s^2$ | 18×18×10 | 450 | 22.896 | 118.607 | 3.805 |
| Ta | $5d^3\ 6s^2$ | 15×15×15 | 120 | 19.039 | 194.423 | 3.890 |
| W | $5s^2\ 5p^6\ 5d^4\ 6s^2$ | 16×16×16 | 120 | 16.084 | 306.980 | 4.566 |
| Re | $5s^2\ 5p^6\ 5d^5\ 6s^2$ | 21×21×11 | 288 | 14.938 | 369.593 | 4.409 |
| Os | $5s^2\ 5p^6\ 5d^6\ 6s^2$ | 21×21×12 | 288 | 14.227 | 399.671 | 5.288 |
| Ir | $5d^7\ 6s^2$ | 13×13×13 | 84 | 14.846 | 367.648 | 5.297 |
| Pt | $5d^9\ 6s^1$ | 13×13×13 | 84 | 15.994 | 255.877 | 5.698 |
| Au | $5d^{10}\ 6s^1$ | 12×12×12 | 56 | 18.355 | 142.702 | 5.306 |
| Hg | $5d^{10}\ 6s^2$ | 12×12×14 | 147 | 29.945 | 9.827 | −0.779 |
| Tl | $5d^{10}\ 6s^2\ 6p^1$ | 16×16×9 | 360 | 31.802 | 26.073 | 4.692 |
| Pb | $5d^{10}\ 6s^2\ 6p^2$ | 10×10×10 | 35 | 32.316 | 34.485 | 4.452 |
| Bi | $6s^2\ 6p^3$ | 13×13×5 | 91 | 35.143 | 45.497 | 4.648 |
| Po | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Rn | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |