Ab initio technicalities

- Density Functional Theory
- Generalized Gradient Corrections[a]
- Projector Augmented Wave Method[b,c]
  - Frozen [Ar] core, $4s^1 3d^7$ in valence
  - Frozen [Ne]$3s^2$ core, $3p^6 4s^1 3d^7$ in valence
  - Calculations with [Ar] potential plus a pair potential correction
- Plane Waves: $\frac{\hbar^2 k^2}{2m} < 300$ eV
- Finite temperature Fermi smearing
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[a] Y. Wang and J. Perdew, Phys. Rev. B, **44**, 13298 (1991).

[b] P. E. Blöchl, Phys. Rev. B, **50**, 17953 (1994); G. Kresse and D. Joubert, Phys. Rev. B, **59**, 1758 (1999).

[c] Our DFT calculations are based on the VASP code, G. Kresse and J. Furthmüller, Comput. Mater. Sci., **6**, 15 (1996); Phys. Rev. B, **54**, 11169 (1996), with the implementation of an efficient charge extrapolation, D. Alfè, Comp. Phys. Comm., **118**, 31-33 (1999).

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