# Supporting information for: Efficient automatized density-functional tight-binding parameterizations: Application to group IV elements

Ahmad W. Huran,[†] Conrad Steigemann,[†] Thomas Frauenheim,[‡] Bálint Aradi,[‡] and Miguel A. L. Marques*,[†]

†*Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06120 Halle (Saale), Germany*

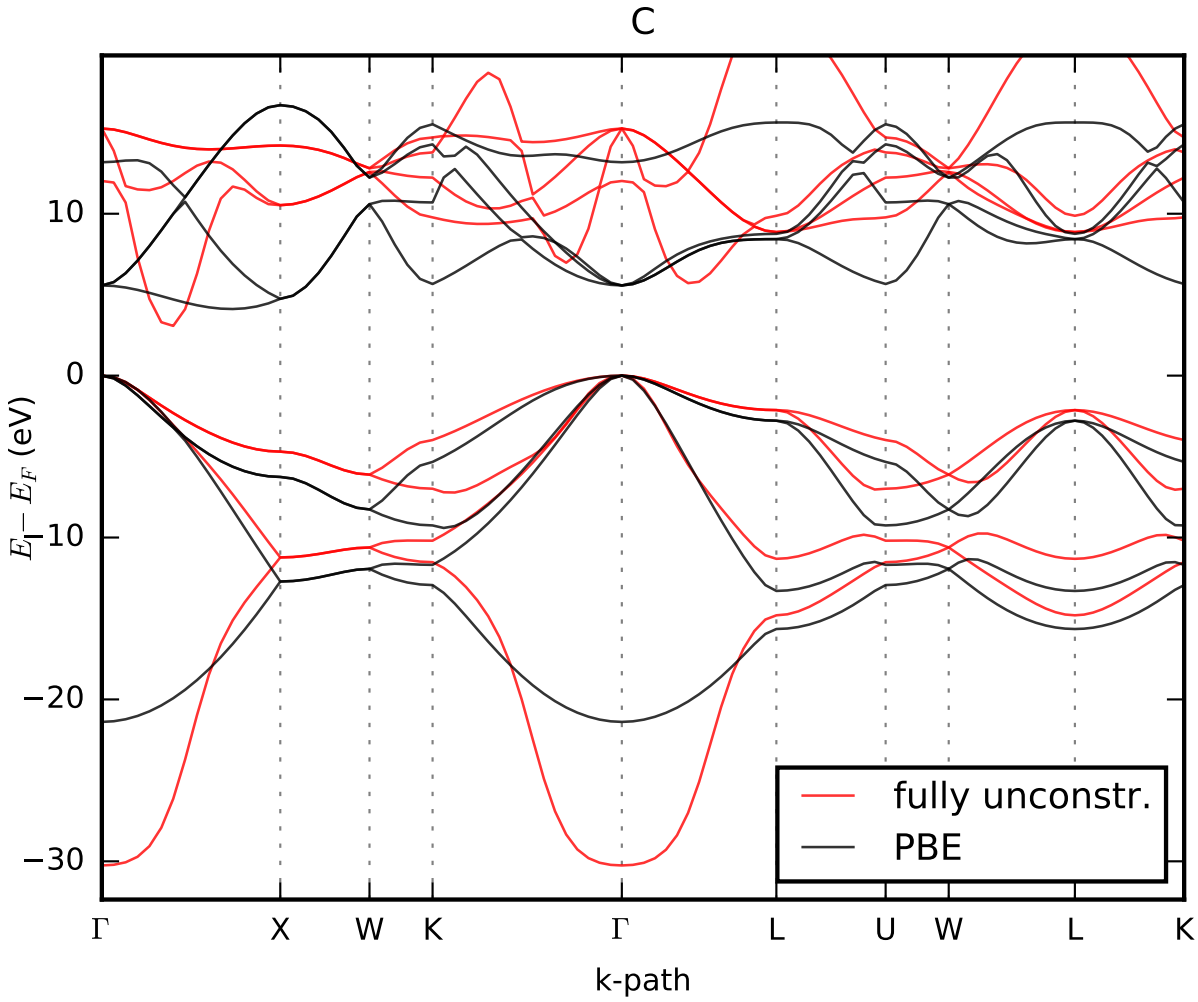
‡*BCCMS, University of Bremen, 28359 Bremen, Germany*

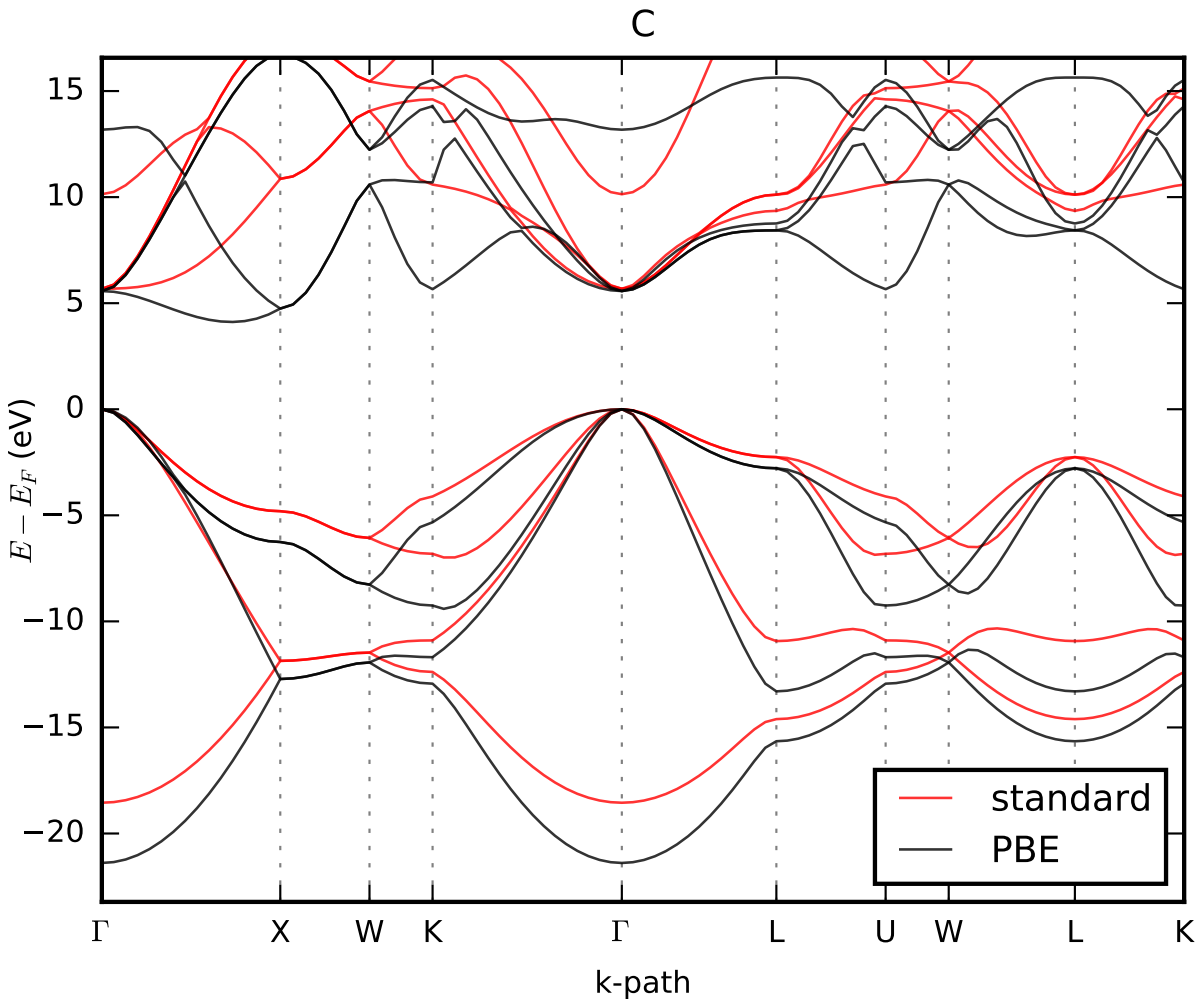
E-mail: miguel.marques@physik.uni-halle.de

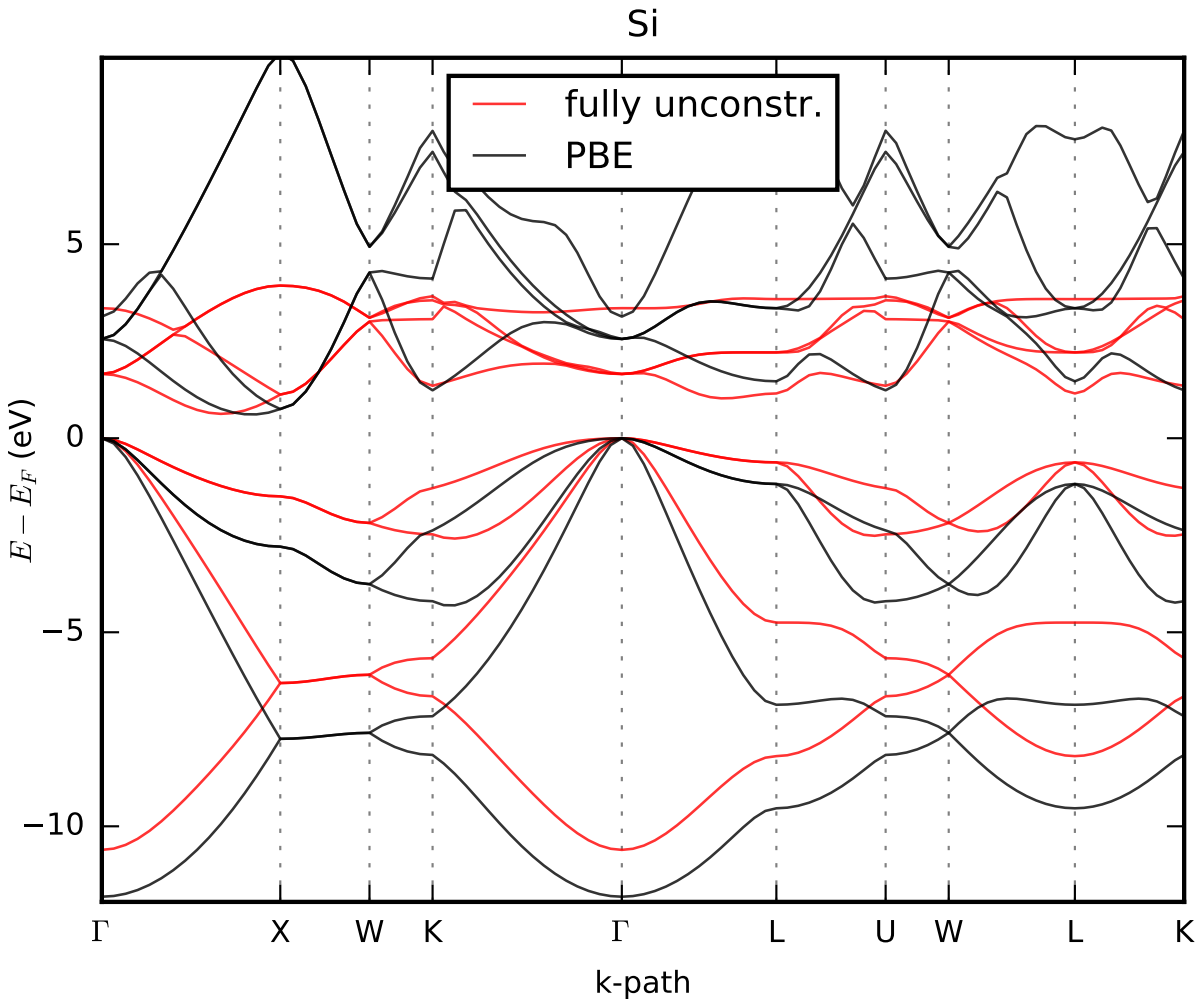
## 1 Introduction

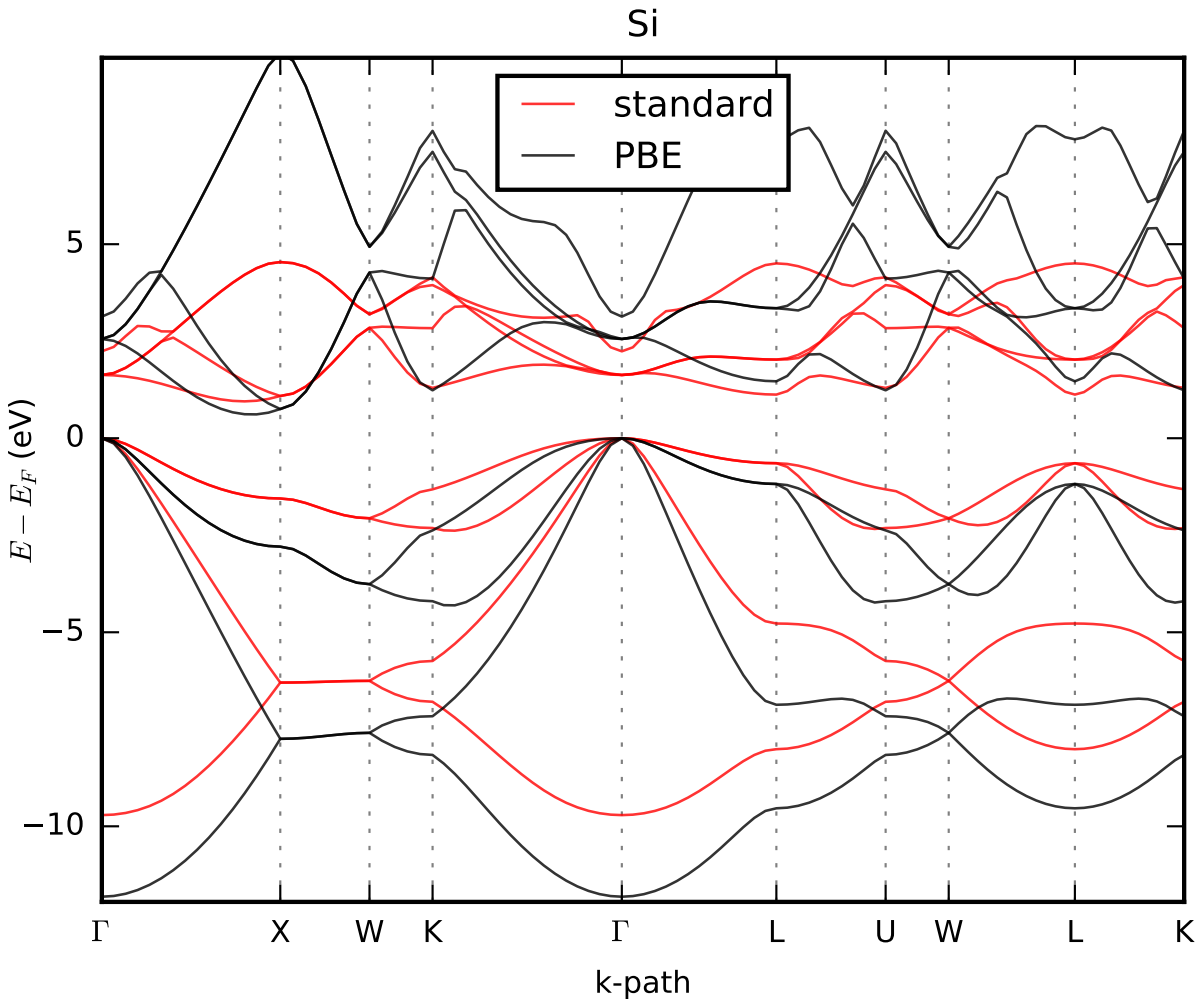
In this document we provide more band structure examples, phonon dispersion curves, bulk moduli, and unit cell volumes. All considered structures are in diamond configuration. For the structures specifications see `structures.zip` in the supplementary material.

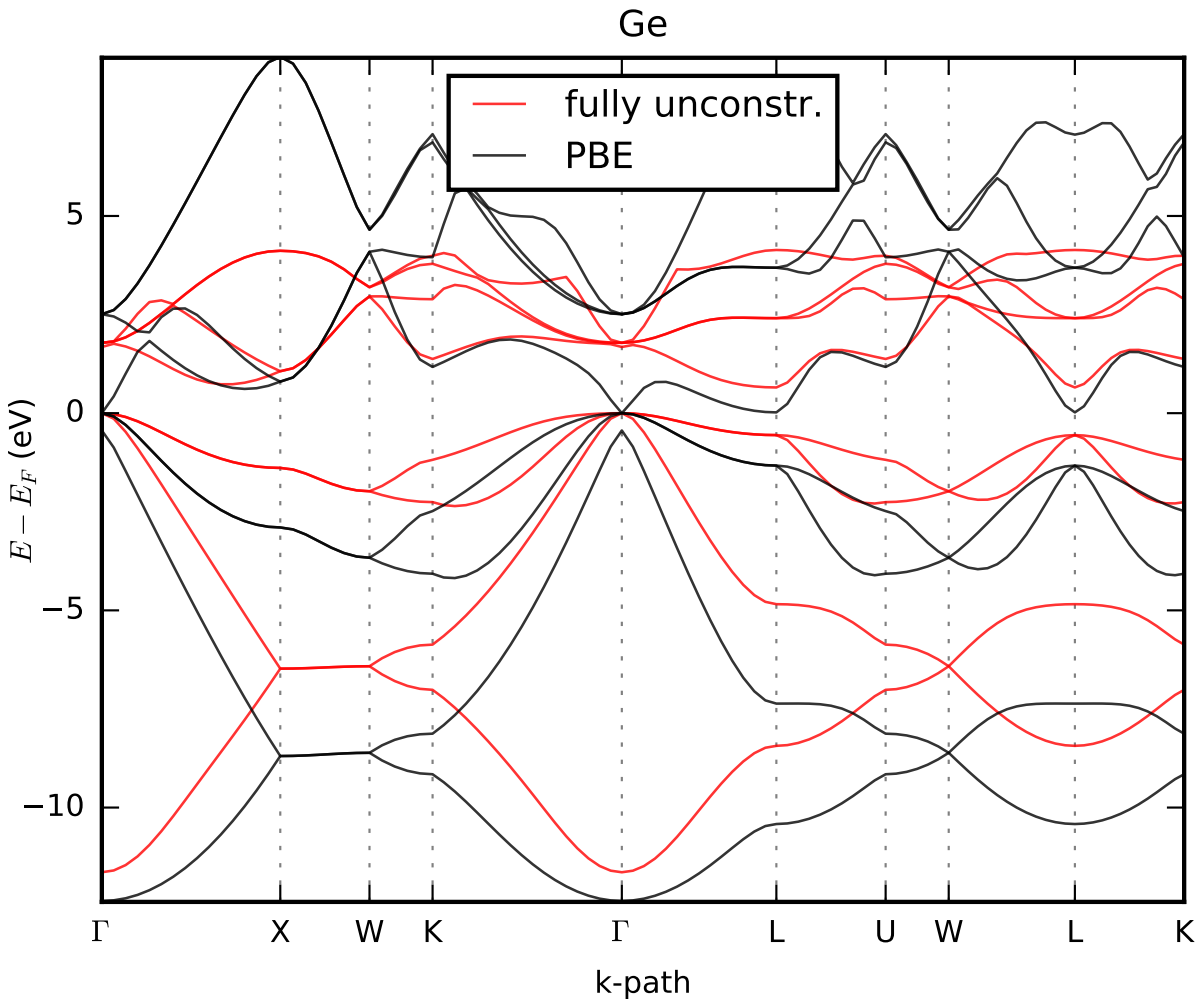
## 2 Band structures

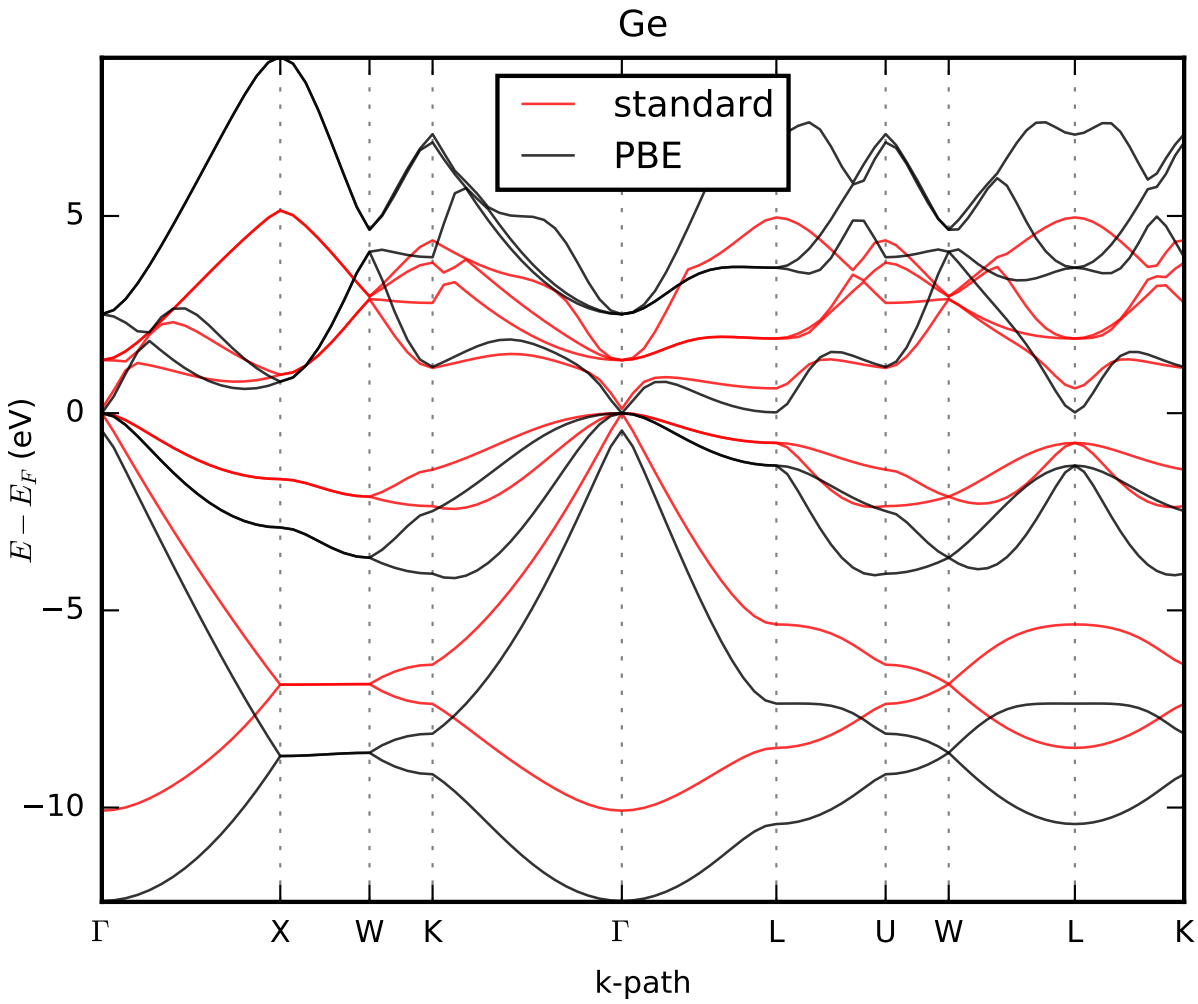


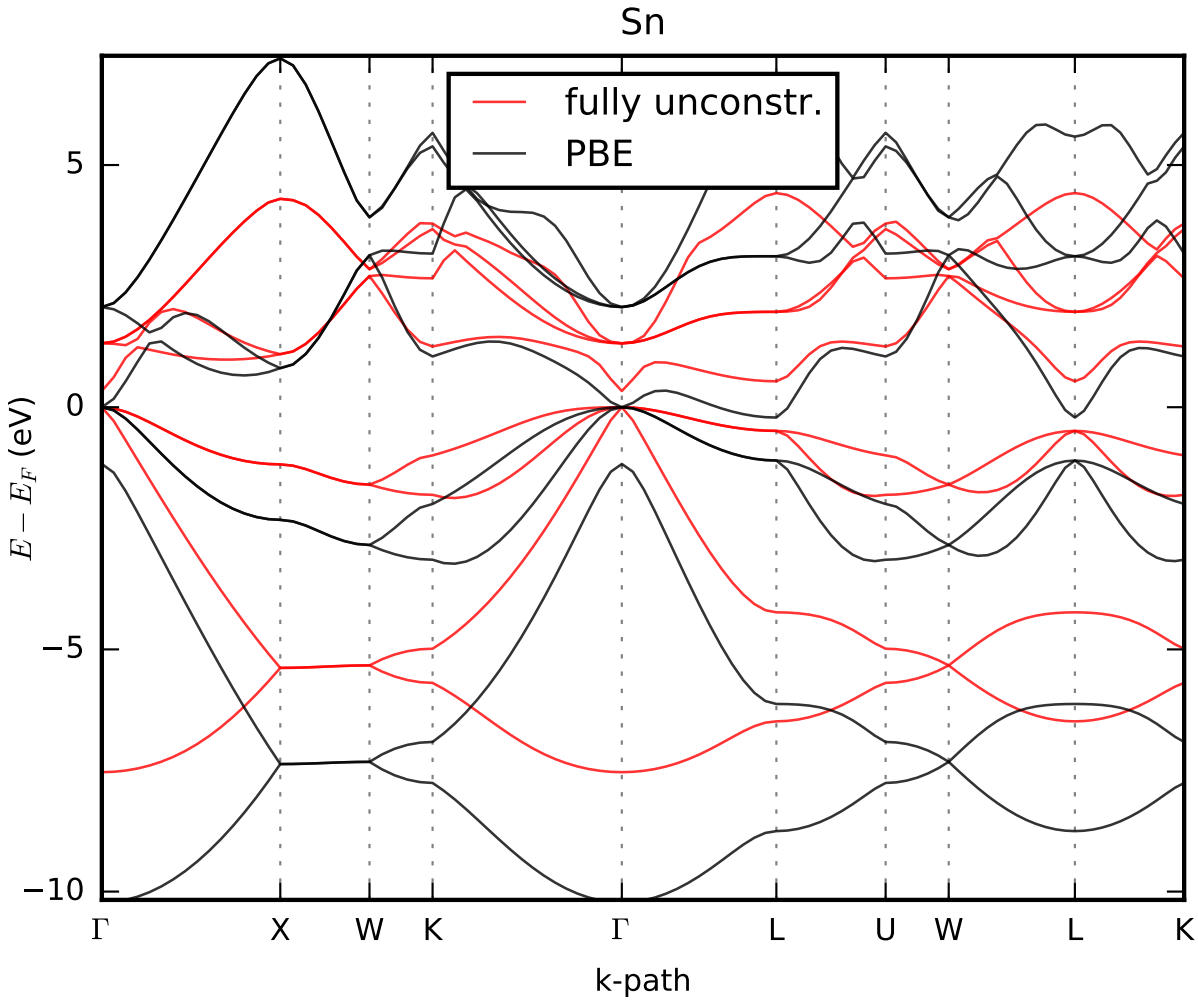

C
15
10
5
0
−5
−10
−15
−20
$E - E_F$ (eV)
Γ
X
W
K
Γ
L
U
W
L
K
k-path
standard
PBE

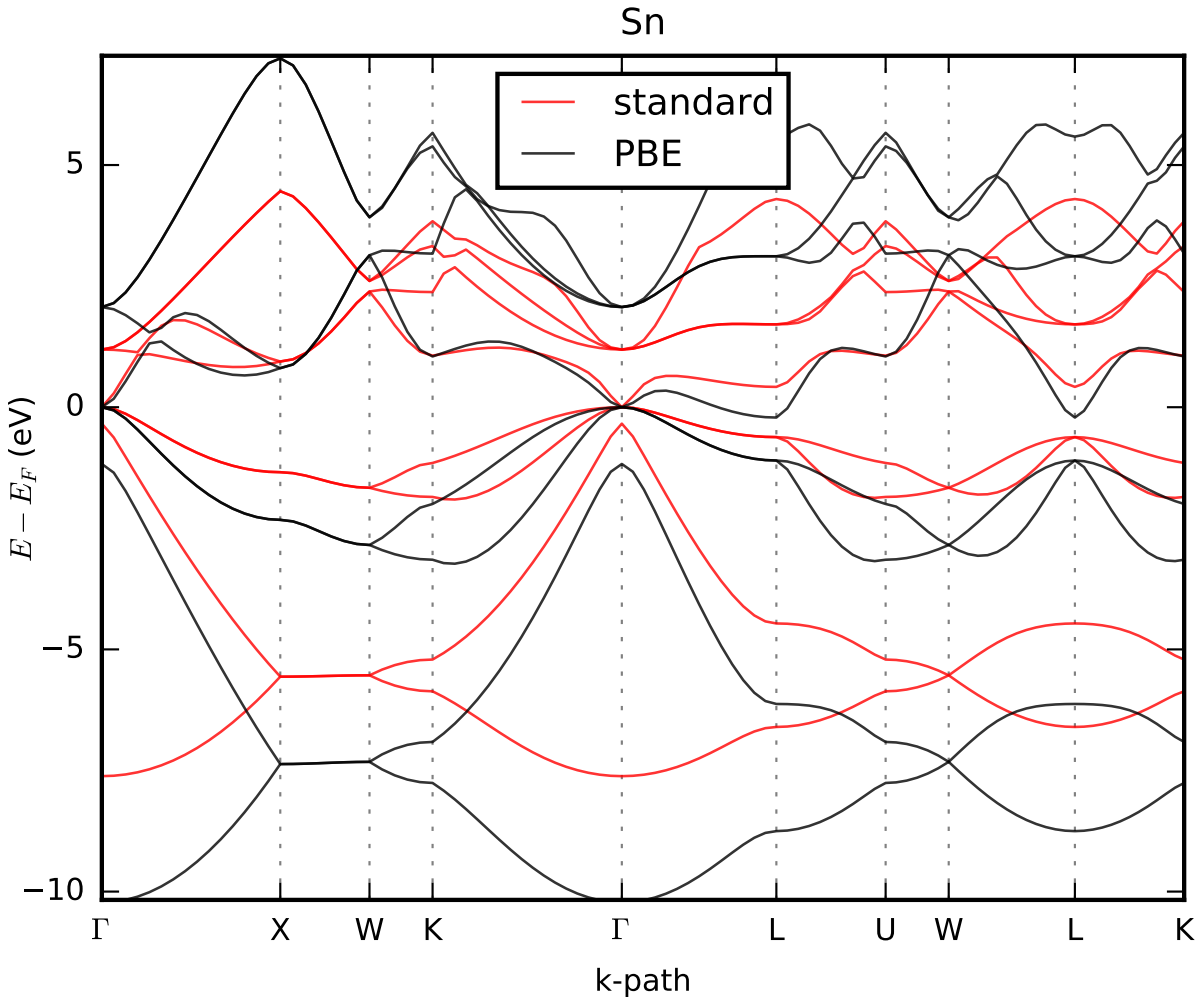

Si
fully unconstr.
PBE
5
0
−5
−10
$E - E_F$ (eV)
Γ
X
W
K
Γ
L
U
W
L
K
k-path


Si
standard
PBE
5
0
−5
−10
$E - E_F$ (eV)
Γ
X
W
K
Γ
L
U
W
L
K
k-path


Ge
fully unconstr.
PBE
5
0
−5
−10
$E - E_F$ (eV)
Γ
X
W
K
Γ
L
U
W
L
K
k-path


Ge
standard
PBE
5
0
−5
−10
$E - E_F$ (eV)
Γ
X
W
K
Γ
L
U
W
L
K
k-path


Sn
fully unconstr.
PBE
5
0
−5
−10
$E - E_F$ (eV)
Γ
X
W
K
Γ
L
U
W
L
K
k-path


Sn
standard
PBE
5
0
−5
−10
$E - E_F$ (eV)
Γ
X
W
K
Γ
L
U
W
L
K
k-path

# 3 Phonon dispersion curves

Phonon dispersion curves were calculated by the finite differences method via the `PHONOPY` package[S1] using 4×4×4 supercells.

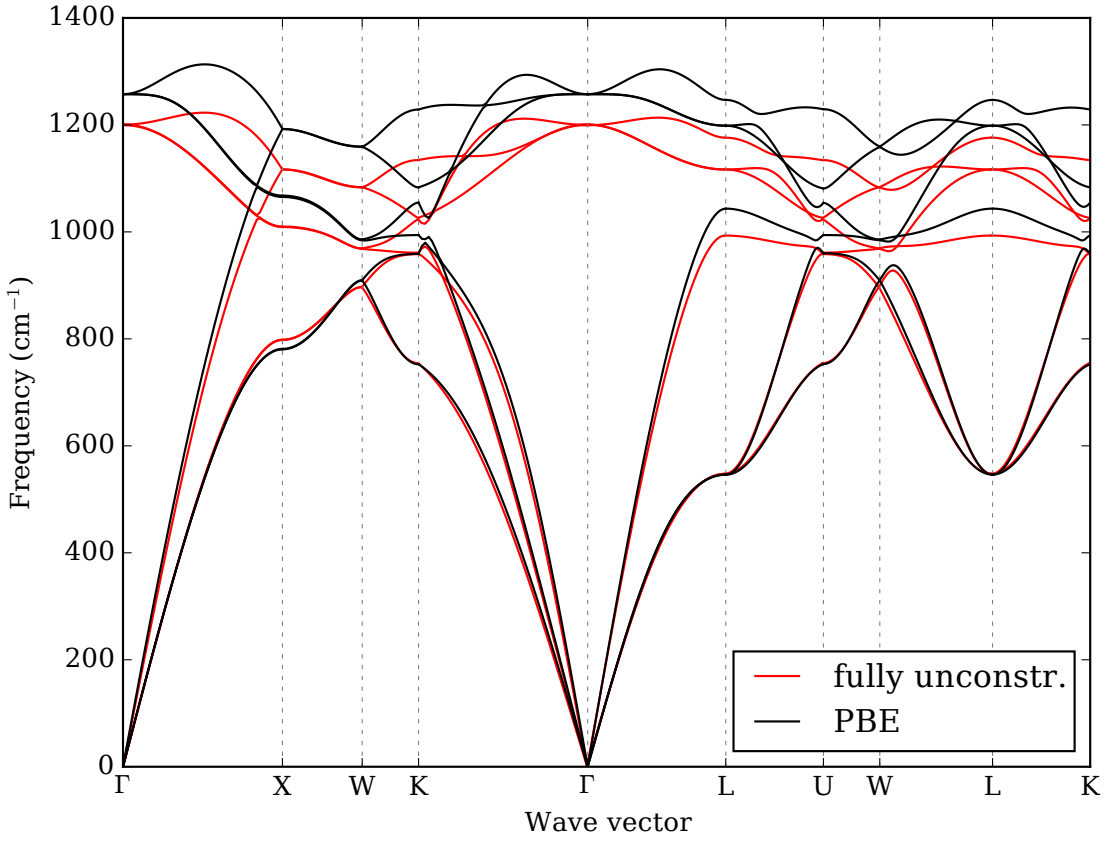



Figure S1: Carbon

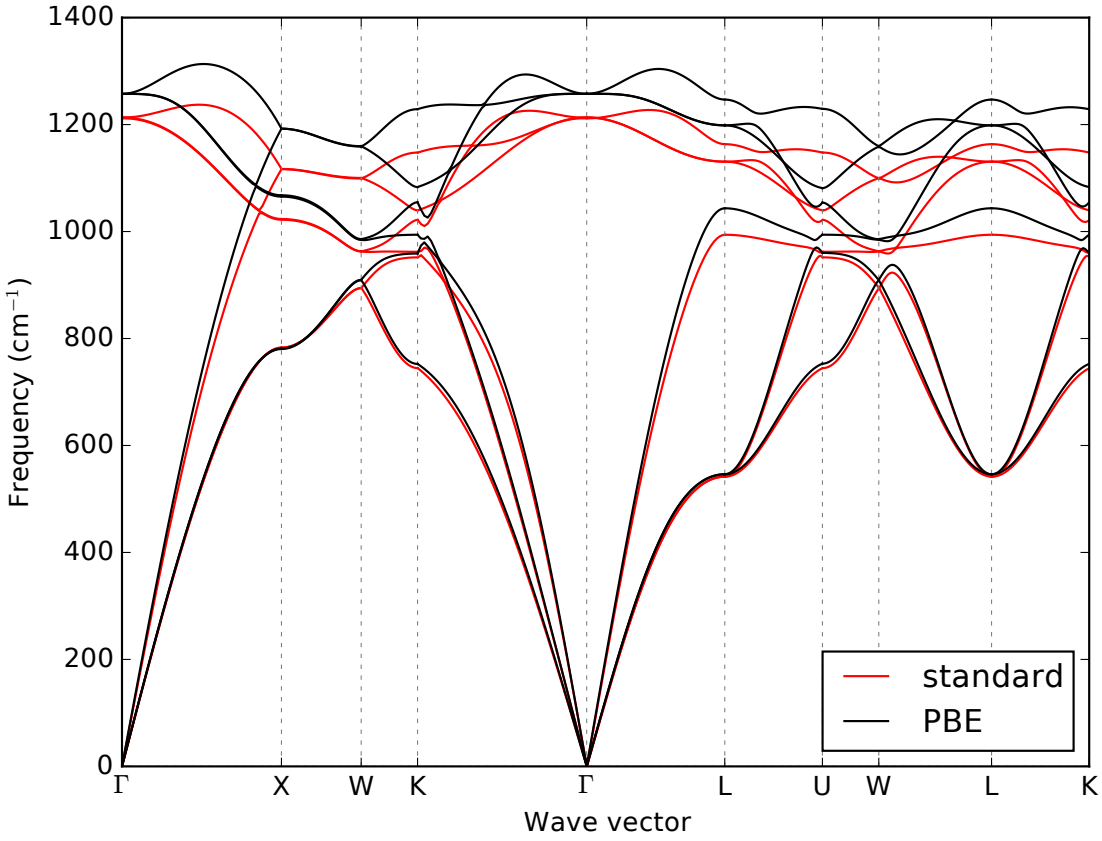



Figure S2: Carbon

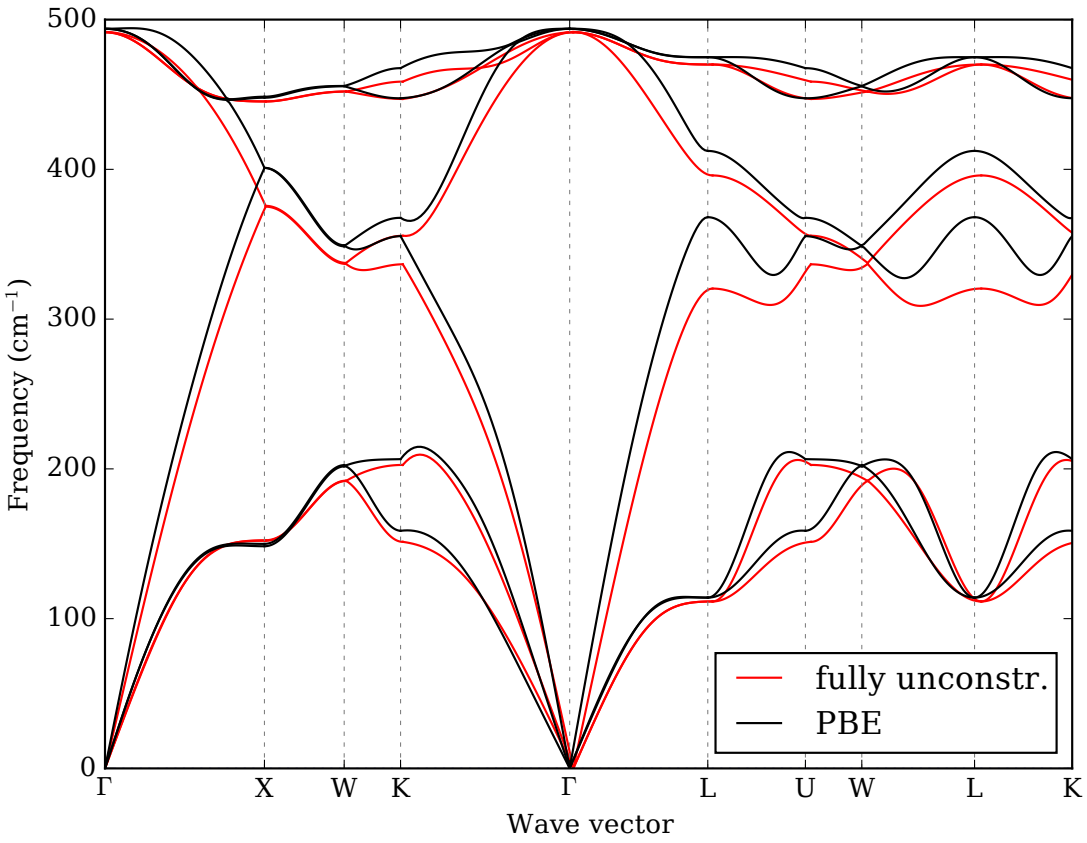



Figure S3: Silicon

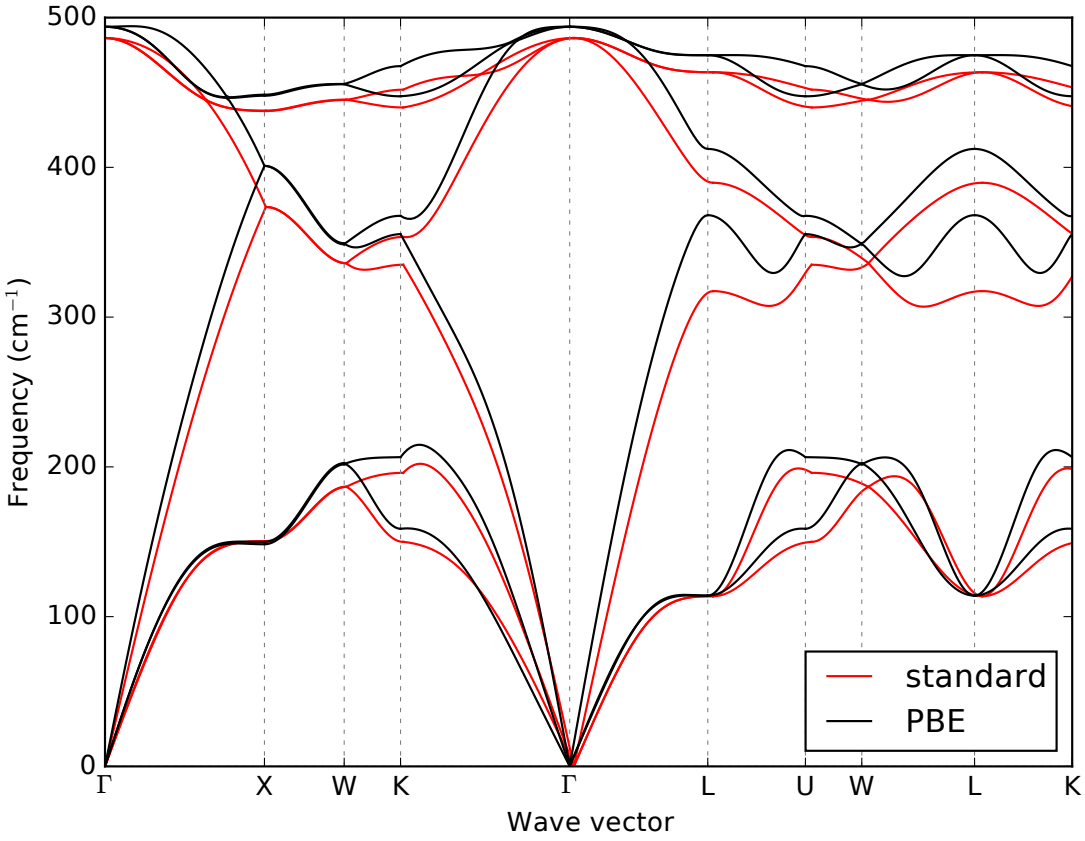



Figure S4: Silicon

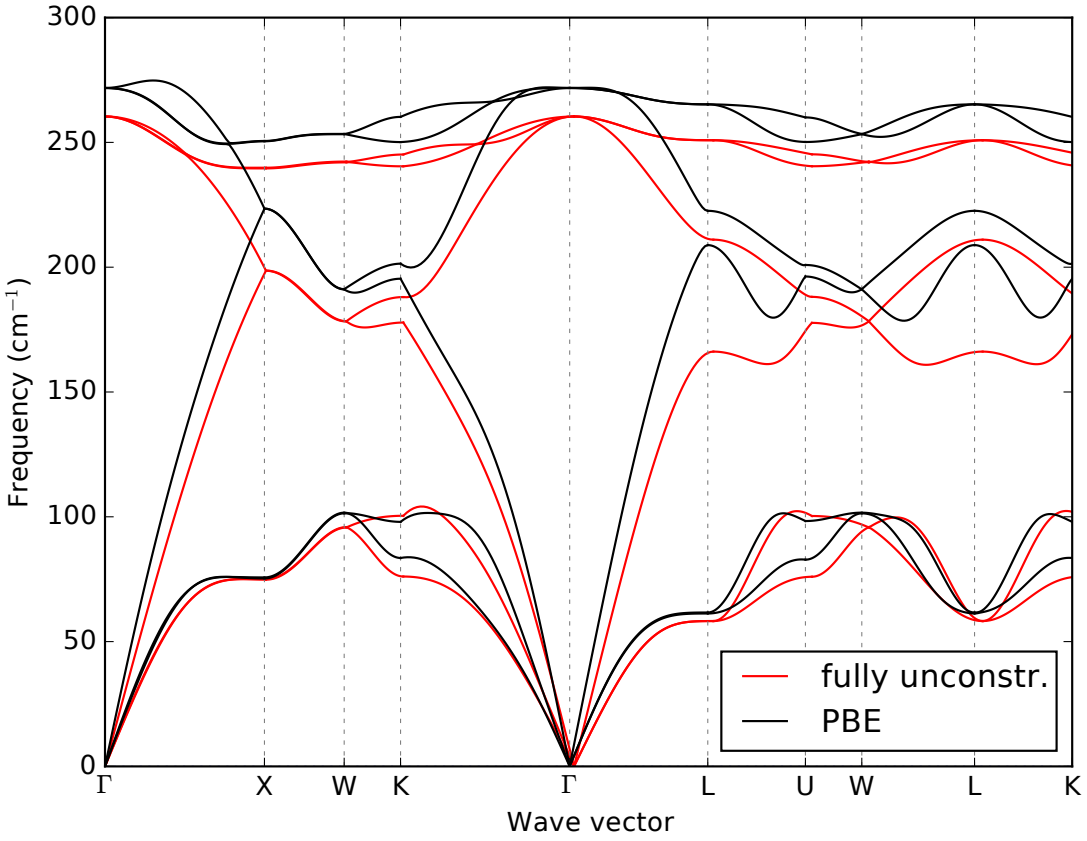



Figure S5: Germanium

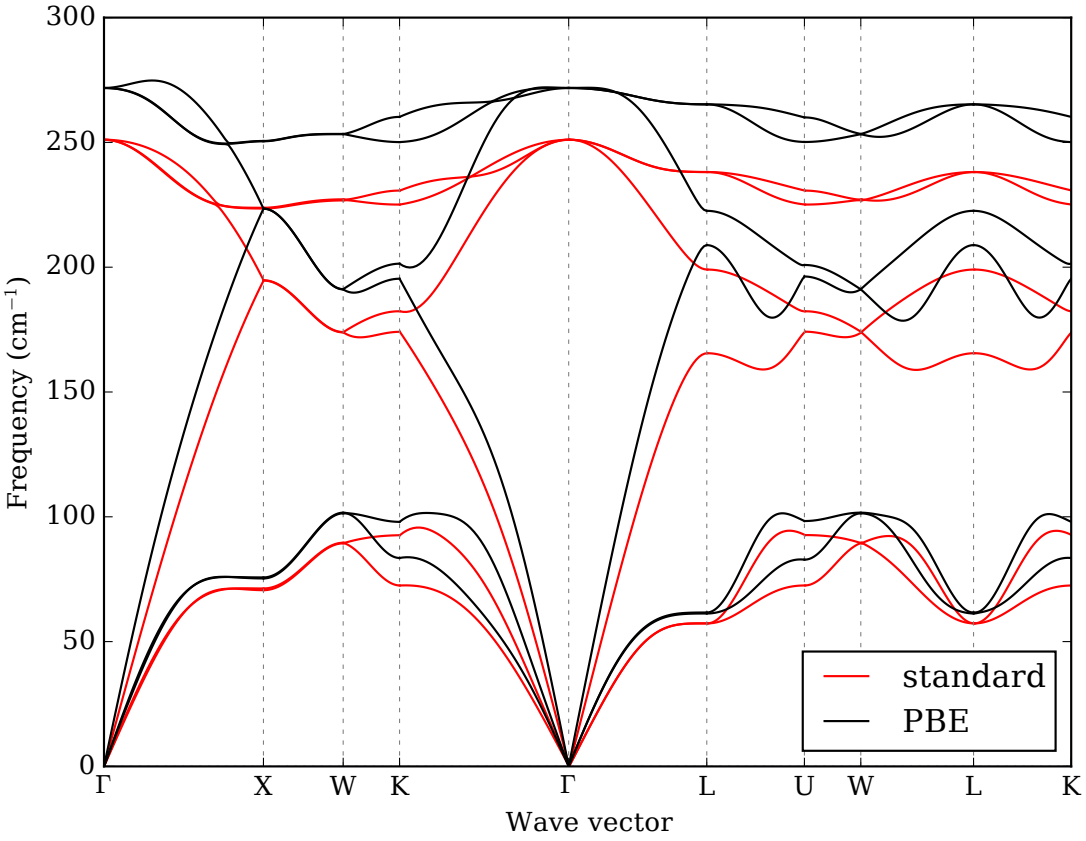



Figure S6: Germanium

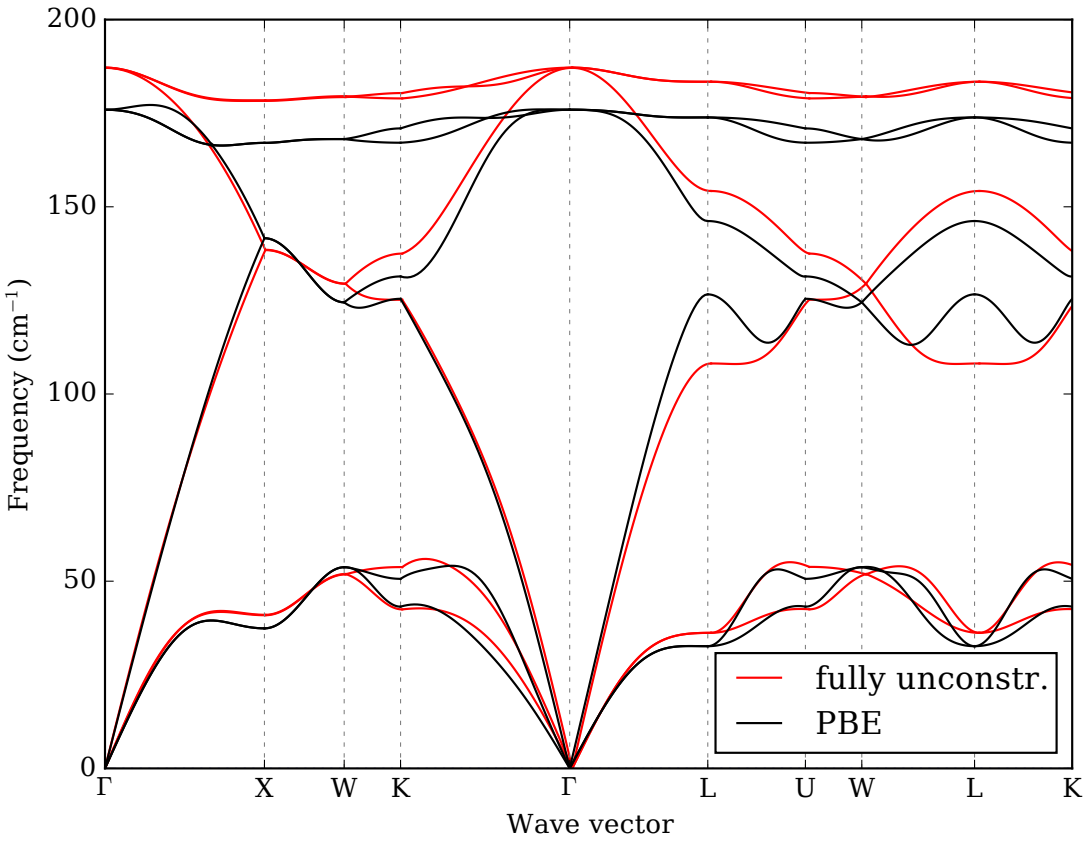



Figure S7: Tin

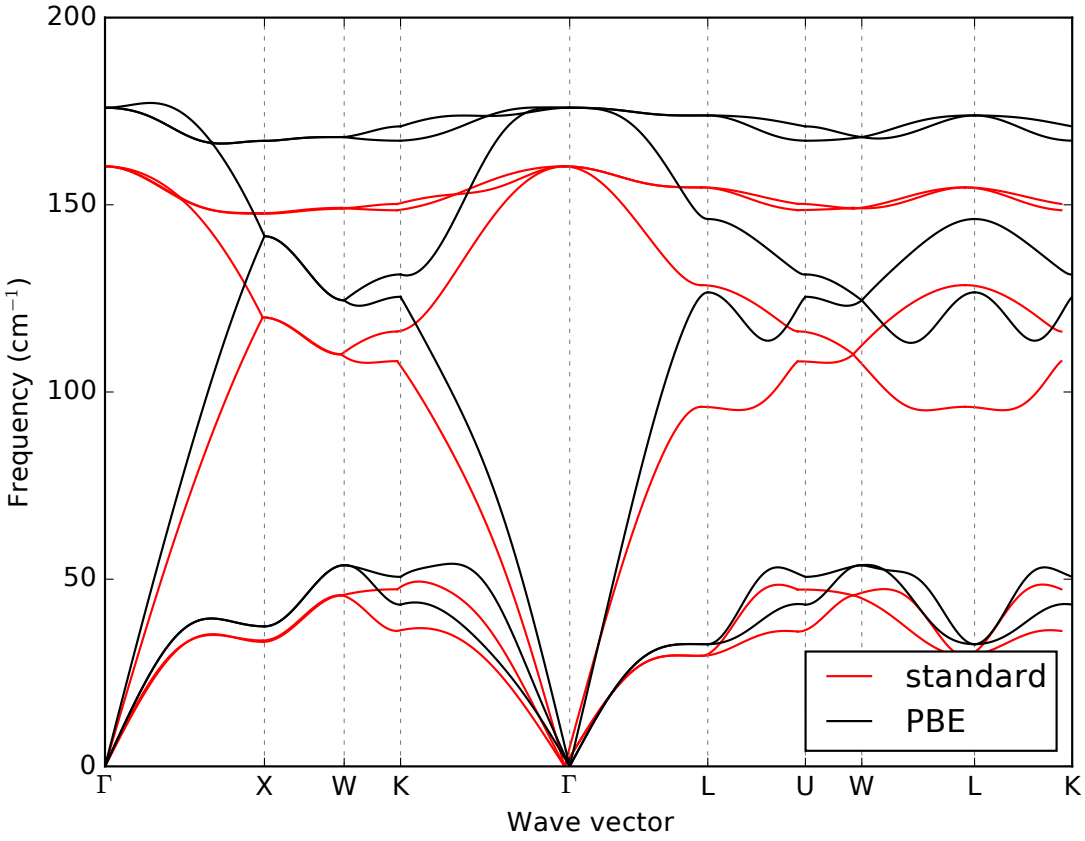



Figure S8: Tin

# 4 Bulk moduli

Table S1: Bulk modulus (GPa) and equilibrium primitive cell volume (Å$^3$) for selected crystal systems in diamond configuration.

| | type | $B$ | $V_0$ |
|---|---|---|---|
| C | PBE | 432.95 | 11.42 |
| | standard | 456.95 | 11.40 |
| | fully unconstr. | 426.96 | 11.46 |
| Si | PBE | 88.77 | 40.89 |
| | standard | 81.66 | 39.81 |
| | fully unconstr. | 83.60 | 39.98 |
| Ge | PBE | 58.82 | 48.36 |
| | standard | 51.20 | 48.37 |
| | fully unconstr. | 56.20 | 47.18 |
| Sn | PBE | 36.32 | 73.57 |
| | standard | 30.79 | 76.13 |
| | fully unconstr. | 41.19 | 72.44 |

# References

(S1) Togo, A.; Tanaka, I. First principles phonon calculations in materials science. *Scr. Mater.* **2015**, *108*, 1–5.