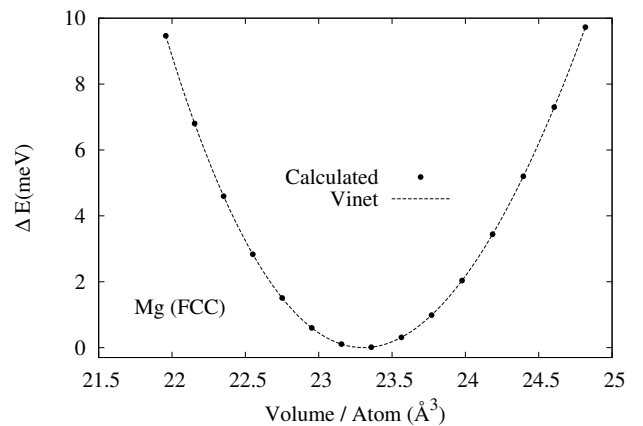
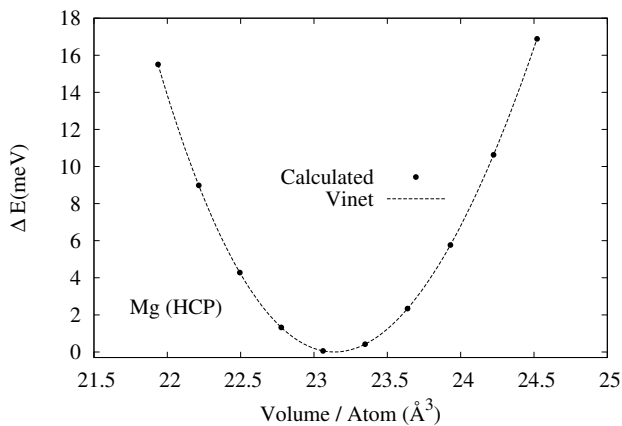
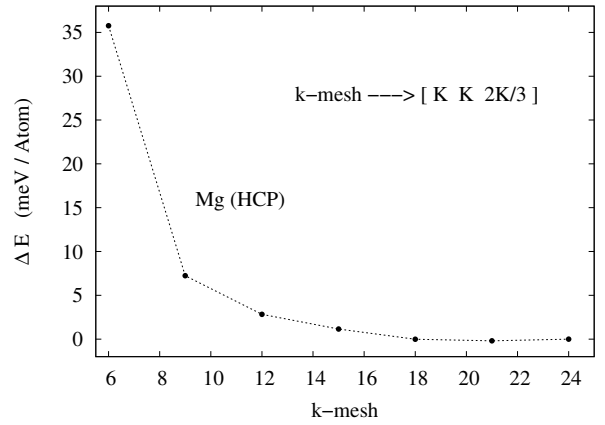
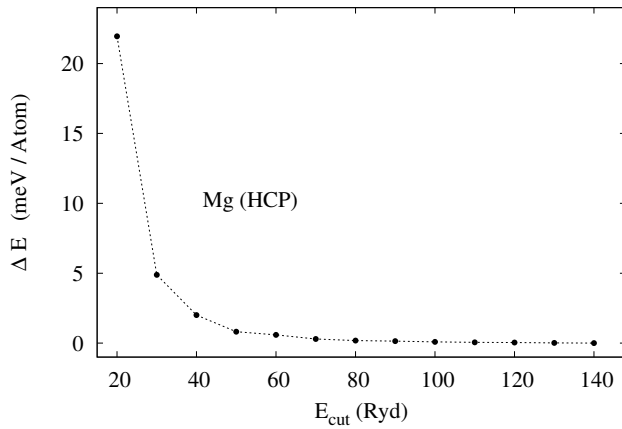


## Some Crude Comparisons for *Mg.GGA-PBE-paw.UPF*

### Calculation Parameters

- $E_{\text{cut}} = 70$  Ryd
- $k_{\text{mesh}} = 12 \times 12 \times 12$  (for Cubic Structures)
- $k_{\text{mesh}} = 12 \times 12 \times 8$  (for Hegzagonal Structures)
- smearing : Marzari-Vanderbilt
- smearing width = 0.01 - 0.02 Ryd
- $\frac{c}{a}$  have been kept constant

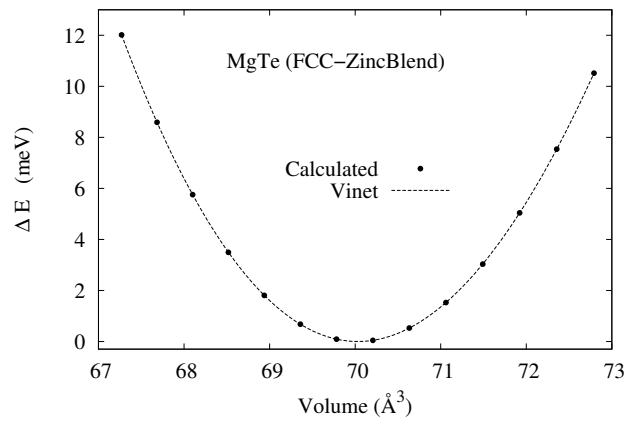
Crystal : Mg		$c/a = (5.21/3.21) = 1.623$ [1]	
	Present (FCC)	Present (HCP)	Exp. (HCP)
Volume / atom ( $\text{\AA}^3$ )	23.304	23.140	23.245
Bulk Modulus (GPa)	35.27	36.274	35.40
dB/dP	4.04	4.12	—



Crystal : MgTe (FCC: ZincBlend)

Te: Te.pbe-rrkj.UPF of Quantum ESPRESSO

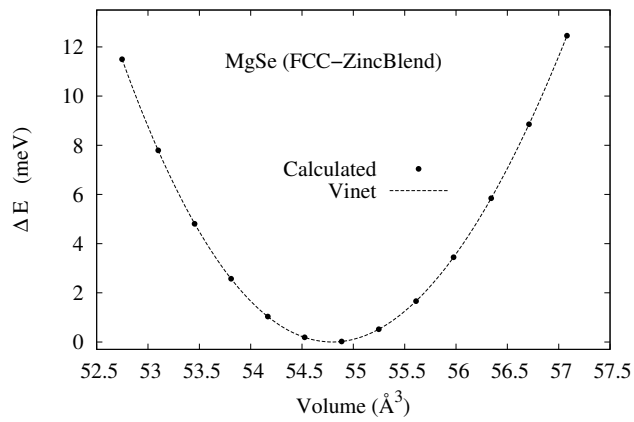
	Present	Theo. [2]	Theo. [3]
Volume ( $\text{\AA}^3$ )	70.031	69.562	64.924
Bulk Modulus (GPa)	33.06	33.80	38.70
dB/dP	4.07	4.31	3.89



Crystal : MgSe (FCC: ZincBlend)

Se: Se.pbe-van.UPF of Quantum ESPRESSO

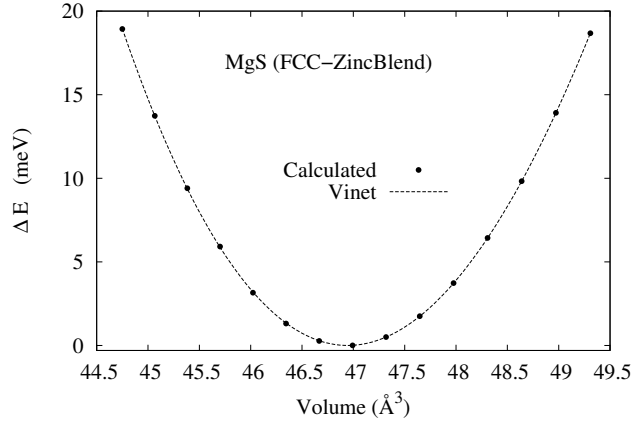
	Present	Theo. [3]
Volume ( $\text{\AA}^3$ )	54.80	50.98
Bulk Modulus (GPa)	44.97	50.50
dB/dP	4.17	4.02



Crystal : MgS (FCC: ZincBlend)

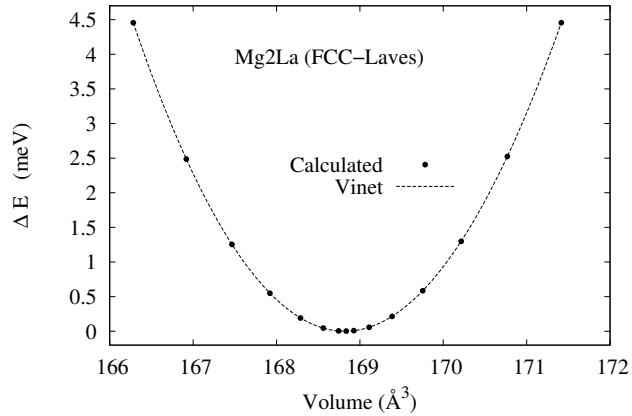
S: S.pbe-van\_bm.UPF of Quantum ESPRESSO

	Present	Theo. [3]
Volume ( $\text{\AA}^3$ )	46.94	44.19
Bulk Modulus (GPa)	54.64	61.20
dB/dP	4.02	4.06

Crystal : Mg<sub>2</sub>La (FCC : Laves)

La: La.GGA-PBE-paw.UPF

	Present	Theo. [4]	Exp. [5]
Volume ( $\text{\AA}^3$ )	168.819	168.689	168.862
Bulk Modulus (GPa)	36.61	36.08	---
dB/dP	3.618	3.635	---



## References

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