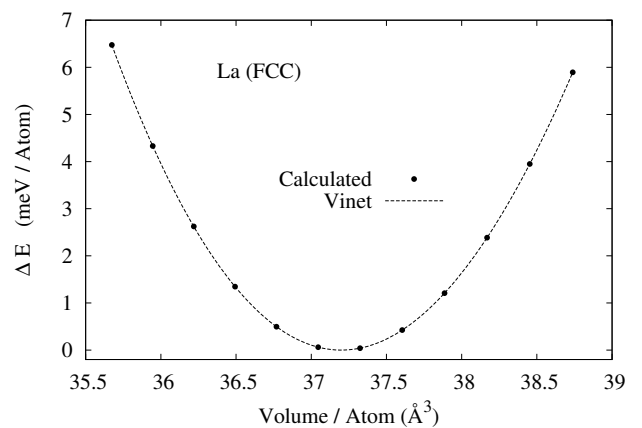
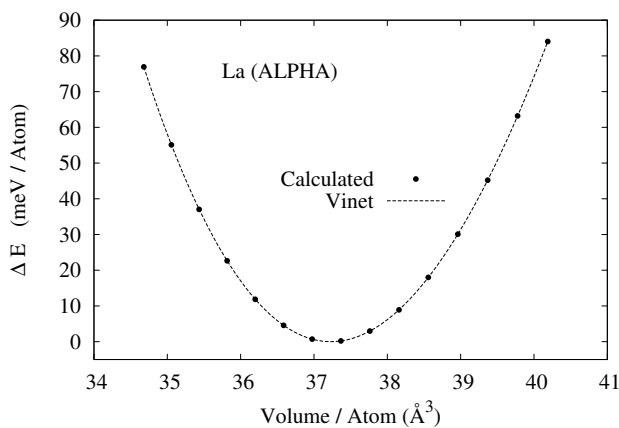
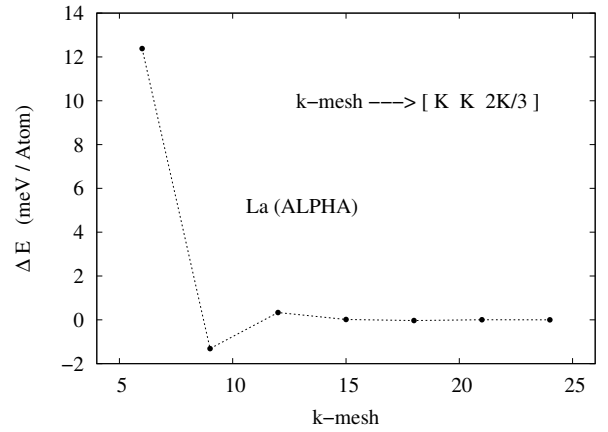
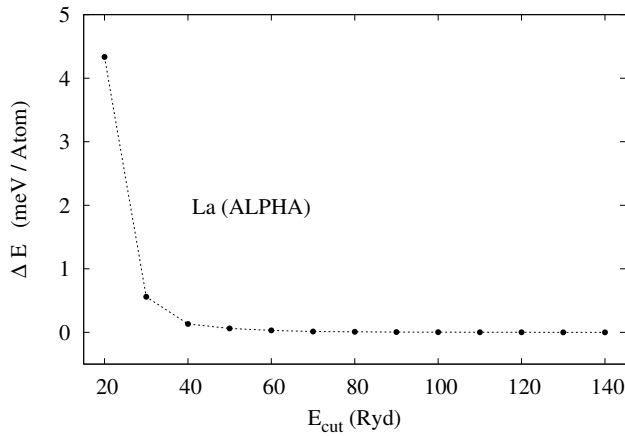


## Some Crude Comparisons for *La.GGA-PBE-paw.UPF*

### 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

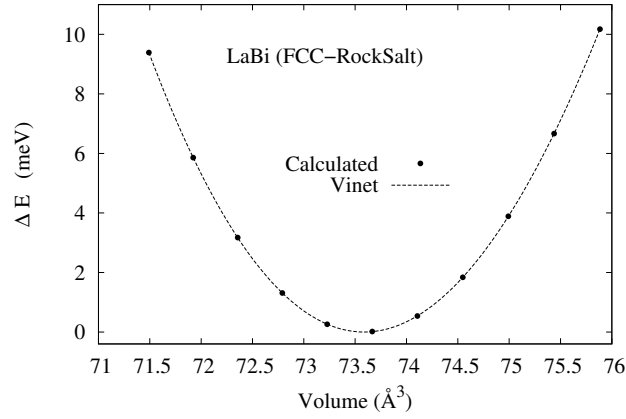
|                                  | Crystal : La  |                 | $c/a = 3.22$ for alpha phase |              |
|----------------------------------|---------------|-----------------|------------------------------|--------------|
|                                  | Present (FCC) | Present (alpha) | Exp. (FCC)                   | Exp. (alpha) |
| Volume / atom ( $\text{\AA}^3$ ) | 37.200        | 37.230          | 37.269 [1]                   | 37.236 [1]   |
| Bulk Modulus (GPa)               | 31.350        | 31.940          | 24.8 [2]                     | 24.3 [3]     |
| dB/dP                            | 3.06          | 3.24            | —                            | —            |



Crystal : LaBi (FCC: RockSalt)

Bi: Bi.pbe-d-mt.UPF of Quantum ESPRESSO

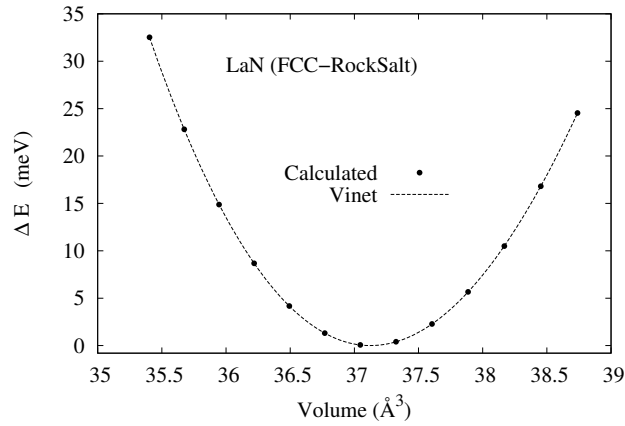
|                           | Present | Theo. [4] | Exp.       |
|---------------------------|---------|-----------|------------|
| Volume ( $\text{\AA}^3$ ) | 73.587  | 74.106    | 70.633 [5] |
| Bulk Modulus (GPa)        | 47.94   | 47.8      | 55.0 [6]   |
| dB/dP                     | 4.26    | 3.95      | —          |



Crystal : LaN (FCC: RockSalt)

N: N.pbe-rrkjus.UPF of Quantum ESPRESSO

|                           | Present | Theo. [4] |
|---------------------------|---------|-----------|
| Volume ( $\text{\AA}^3$ ) | 37.1258 | 36.935    |
| Bulk Modulus (GPa)        | 120.518 | 119.7     |
| dB/dP                     | 4.03    | 4.39      |



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