Evaluate the total Berry phase for each of two calculations performed

$$\phi = \phi_{\mathrm{el}} + \phi_{\mathrm{ion}}$$

and its change

$$\Delta\phi = \phi(\mathrm{perturbed}) - \phi(\mathrm{unperturbed})$$

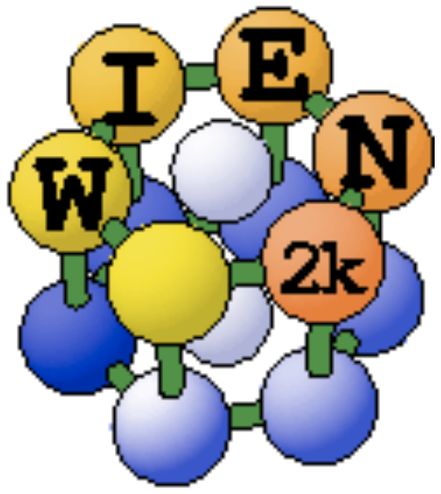
Compute the effective charge Z* of Nitrogen in GaN using a Berry phases and the "shortcut" expression

$$Z^*_{ii} = \frac{\Delta\phi_i}{2\pi\Delta u_i}$$

Here Δu is the displacement in fractional coordinates. The equation applies to the case of one atom displaced. In our case, we need to take into account that 2 N-atoms were shifted.

Compare computed Z* with the literature value of -2.73 [Volume 44D of the series Landolt-Börnstein - Group III Condensed Matter pp 420-423, "GaN: effective charge, dielectric constants" by D. Strauch]

Effective band structure of $Si_{1-x}Ge_x$ alloy



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YouTube video: