The formation energy of an isolated defect equals the formation energy of a defect calculated from DFT calculation minus the elastic correction energy.

$$E_{F,iso} = E_{F,DFT} - E_{el}^{corr}$$

Elastic correction energy has two parts. The first part is the dipole-dipole interactions with periodic images. The second part is the averaged strain correction.

$$E_{el}^{corr} = E_{DD} + E_{strain}^{corr}$$

The dipole-dipole interactions has two parts again.

$$E_{DD} = E_{DD}^{total} + E_{DD}^{corr}$$

$$E_{DD}^{total} = \frac{1}{2} P_{ij} P_{kl} \sum_{n \neq 0} G_{ik,jl}(\boldsymbol{R}_n)$$

$$E_{DD}^{corr} = \frac{-1}{2V_{cell}} P_{ij} P_{kl} \int_{V_{cell}} \sum_{n \neq 0} G_{ik,jl}(\boldsymbol{R}_n - \boldsymbol{r})\, dV$$

Apply divergence theorem,

$$E_{DD}^{corr} = \frac{-1}{2V_{cell}} P_{ij} \int_S G_{ik,j}(\boldsymbol{R}_n - \boldsymbol{r}) P_{k\alpha} n_\alpha dS$$

The averaged stain correction.

$$E_{strain}^{corr} = \frac{-1}{2} \int_{V_{cell}} \sigma_{ij} \bar{\epsilon}_{ij}^{D} dV$$

$$= \frac{1}{2} P_{ij} \bar{\epsilon}_{ij}^{D}$$

$$= \frac{1}{2} P_{ij} \frac{1}{V_{cell}} \int_{V_{cell}} \epsilon_{ij}^{D}(\boldsymbol{r}) dV$$

$$= \frac{1}{2} P_{ij} \frac{1}{V_{cell}} \int_{V_{cell}} \left(-G_{ik,jl}(\boldsymbol{r}) P_{kl}\right) dV$$

$$= \frac{-1}{2V_{cell}} P_{ij} \int_{V_{cell}} G_{ik,jl}(\boldsymbol{r}) P_{kl} dV$$

Apply divergence theorem,

$$= \frac{-1}{2V_{cell}} P_{ij} \int_S G_{ik,j}(\boldsymbol{r}) P_{k\alpha} n_\alpha dS$$

It helps avoiding $\boldsymbol{r} = \boldsymbol{0}$.