Virial (dimer in a box)

$$v_{\alpha\beta} = -\frac{1}{2}\sum_{M=1}^{2}\sum_{N\neq M}^{2}(R_M^\alpha - R_N^\alpha)F_M^\beta \tag{1}$$

Virial Stress

$$\tau_{\alpha\beta} = -\frac{1}{2\Omega}\sum_{M}\sum_{\bar{L}\in\mathcal{N}(M)}(R_M^\alpha - R_{\bar{L}}^\alpha)F^\beta_{M\leftarrow\bar{L}} \tag{2}$$

HFX

$$\begin{aligned}
F_M^\beta &= -\frac{\partial E_\Gamma^{x,\mathrm{TCI}}}{\partial R_M^\beta} && (3)\\
&= \frac{1}{2}\sum_{\mu[M]}\sum_{N\neq M}\sum_{\nu[N]}\left[\partial_{R_M^\beta}\mathbf{S}(\Gamma)\right]_{\mu\nu}\underbrace{\left[\mathbf{\Delta P S}\left(\mathbf{\Delta P}\odot\tilde{\gamma}^{\mathrm{TCI}}\right)+\left((\mathbf{\Delta P S})\odot\tilde{\gamma}^{\mathrm{TCI}}\right)\mathbf{\Delta P}\right]^{\mathrm{sym}}_{\nu\mu}}_{[\mathbf{V}^{(1)}]_{\nu\mu}\equiv V^{(1)}_{\nu\mu}}\\
&+\frac{1}{4}\sum_{\mu[M]}\sum_{N\neq M}\sum_{\nu[N]}\left[\partial_{R_M^\beta}\tilde{\gamma}^{\mathrm{TCI}}\right]_{\mu\nu}\underbrace{\left[(\mathbf{\Delta P S})\odot(\mathbf{\Delta P S})^\top+(\mathbf{S\Delta P S})\odot\mathbf{\Delta P}\right]_{\nu\mu}}_{[\mathbf{V}^2]_{\nu\mu}\equiv V^{(2)}_{\nu\mu}}, && (4)\\
&= \frac{1}{2}\sum_{\mu\nu}^{\mathrm{u.c.}}\Big[\sum_{\bar{N}\in\mathcal{N}(M)}\partial_{R_M^\beta}S_{\bar{\nu}\mu}\Big]_{\nu\mu}V^{(1)}_{\nu\mu}+\frac{1}{4}\sum_{\mu\nu}^{\mathrm{u.c.}}\Big[\sum_K\sum_{\mathbf{g}}\partial_{R_M^\beta}\gamma^{\mathrm{TCI}}_{K[\mathbf{g}]M}\Big]_{\nu\mu}V^{(2)}_{\nu\mu} && (5)
\end{aligned}$$

$$\begin{aligned}
\tau_{\alpha\beta} &= -\frac{1}{4\Omega}\Big\{\sum_{\mu[M]}\sum_{M}\sum_{\nu[N]}\sum_{N}\Big[\sum_{\bar{L}\in\mathcal{N}(M)}(R_M^\alpha - R_{\bar{L}}^\alpha)\partial_{R_M^\beta}S\Big]_{\mu\nu}V^{(1)}_{\nu\mu}\\
&+\frac{1}{2}\sum_{\mu[M]}\sum_{M}\sum_{\nu[N]}\sum_{N}\Big[\sum_K\sum_{\mathbf{g}}(R_M^\alpha - R^\alpha_{K[\mathbf{g}]})\partial_{R_M^\beta}\gamma^{\mathrm{TCI}}(\mathbf{g})\Big]_{\mu\nu}V^{(2)}_{\nu\mu}\Big\}, && (6)\\
&= -\frac{1}{4\Omega}\Big\{\sum_{M}\sum_{\mu\nu}^{\mathrm{u.c.}}\Big[\sum_{\bar{N}\in\mathcal{N}(M)}(R_M^\alpha - R^\alpha_{\bar{N}})\partial_{R_M^\beta}S_{\bar{\nu}\mu}\Big]_{\nu\mu}V^{(1)}_{\nu\mu}+\frac{1}{2}\sum_{M}\sum_{\mu\nu}^{\mathrm{u.c.}}\Big[\sum_K\sum_{\mathbf{g}}(R_M^\alpha - R^\alpha_{K[\mathbf{g}]})\partial_{R_M^\beta}\gamma^{\mathrm{TCI}}_{K[\mathbf{g}]M}\Big]_{\nu\mu}V^{(2)}_{\nu\mu}\Big\} && (7)
\end{aligned}$$

DFTB1

$$\tau_{\alpha\beta} = -\frac{1}{2\Omega}\sum_{M}\sum_{\bar{L}\in\mathcal{N}(M)}\sum_{\mu[M]}\sum_{\bar{\lambda}[\bar{L}]}\left[R_M^\alpha - R_{\bar{L}}^\alpha\right]\left[P_{\bar{\lambda}\mu}\partial_{R_M^\beta}H^{(0)}_{\bar{\lambda}\mu} - P^{\mathrm{e}}_{\bar{\lambda}\mu}\partial_{R_M^\beta}S_{\bar{\lambda}\mu}\right] \tag{8}$$