Density Functional Perturbation Theory

Pietro Delugas
SISSA, Trieste

SISSA

QUANTUMESPRESSO

MAX DRIVING THE EXASCALE TRANSITION

- DFPT is a method for computing the derivative of the ground state density with respect to the external parameters of the KS Hamiltonian.
- Powerful tool for computing derivatives up to third order

$$H_{KS} = -\frac{\hbar^2}{2m}\nabla_r^2 + e^2 \int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3r' + v_{xc}[n](\mathbf{r}) - \sum_{iI} \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|}$$

Interatomic Force Constants

Force derivative with respect to atomic displacements: $$L^{\beta,k'}_{\alpha,k} = \frac{\partial F_{\alpha,k}}{\partial u_{\beta,k'}}$$