

electronic density

$$\mathbf{n}(\mathbf{r})$$

**DFT**



1<sup>st</sup>-order  
density matrix

$$\mathbf{P}^{(1)}$$

1<sup>st</sup>-order density

$$\mathbf{n}^{(1)}(\mathbf{r})$$

1<sup>st</sup>-order total  
electrostatic  
potential

$$\mathbf{V}_{es,tot}^{(1)}(\mathbf{r})$$

**DFPT**

1<sup>st</sup>-order  
Hamiltonian

$$\mathbf{H}^{(1)}$$

1<sup>st</sup>-order expansion  
coefficients

$$U^{(1)}(\mathbf{k})$$

Polarizability

$$\alpha$$

