

Molecular Dynamics: 10-30 ... 1000 time steps

$$\mathbf{F} = -\frac{\partial}{\partial \mathbf{R}}(E_{Ewald} + E[n])$$

Electronic Self-consistency: 15-50 steps

$$E[n] = T_0[n] + E_{ext}[n] + E_H[n] + E_{xc}[n]$$

For each \mathbf{k} of the Brillouin Zone: 1-10 ... 10,000 kpts

Diagonalization of the Hamiltonian

$$\sum_{n'} (H_{\mathbf{k}}^{n,n'} - \varepsilon_{\mathbf{k}\nu} S_{\mathbf{k}}^{n,n'}) c_{\mathbf{k}\nu}^{n'} = 0$$

↪ **electronic eigenstates**

↪ **Electronic density;** forces on ions

↪ **Minimum** of total Energy (Correlation functions)

