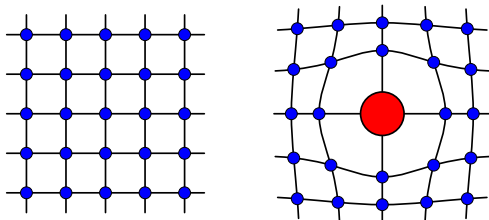# Lattice Relaxation Problems

Given an **energy** $\mathcal{E}$ from an **atomistic/electronic structure** model, solve

> ### Minimisation Problem
> $$u \in \mathrm{argmin}_{v \in \mathcal{H}} \mathcal{E}(v) - \mathcal{E}(0)$$

Main Results:

1. Problem is **well-posed** for **electronic structure** models.
2. **Decay** of minimisers - $|Du(\ell)| \lesssim |\ell|^{-2}$ for **point defects** in $\mathbb{R}^3$.
3. Applications - Neutrality of point defect systems in the **TFW** model.