Lattice Relaxation Problems

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

$$u \in \arg\min_{v \in H} \mathcal{E}(v) - \mathcal{E}(0)$$

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.