Make initial structures Update database Train model Mutate population  $m \cdot t_{ML}$  $x^{(i-1)} \quad x^{(i)}$  $r^{(i+1)}$  $r^{(N_c-1)} r^{(N_c)}$ E Energy Fitness **₹ ₹**  $x^{(best)} - \bullet$ DFT  $E_{\text{best}}$ ,  $(x_{\text{dp}}, E_{\text{dp}})$