

Top track: direct
reparameterization using
experimental data on designs

Bottom track: use experimental
data on designs to identify
problems; reparameterization on
high-quality benchmarks

Experimental data
on designs



Detect recurrent
failure mode



e.g., steric clashing



Update energy
function



Identify corresponding
failure in high-quality
benchmarks



*e.g., relaxing high-
resolution crystal structures*