

INPUTS

Molecular Structure $\hat{\Omega}(\mathbf{k})$

Pair Potentials $U(\mathbf{r})$

Composition ρ_α

Initial Guess $\Gamma(\mathbf{r})$

Closure Expressions

Optimization Routine

PRISM Cost
Function
Kernel

OUTPUTS

Total Correlations $H(\mathbf{r})$

Direct Correlations $C(\mathbf{r})$