Crystal Structure

r

Crystal Graph

$\Rightarrow$

Atomic Numbers
$\{Z_i\}$

Interatomic Radii
$\{\vec{r}_{ab}\}$

Embedding

RBF

$3\times\Big\{$ Equivariant Convolution

Self-Interaction

Pooling

$\{\hat{Y}_m^\ell\}$
Spherical Harmonic
Tensor Components

Dielectric

$$\epsilon_{ij} = \frac{1}{3} s g_{ij} + R_{ij}$$

$(\ell = 0)$

$(\ell = 2)$