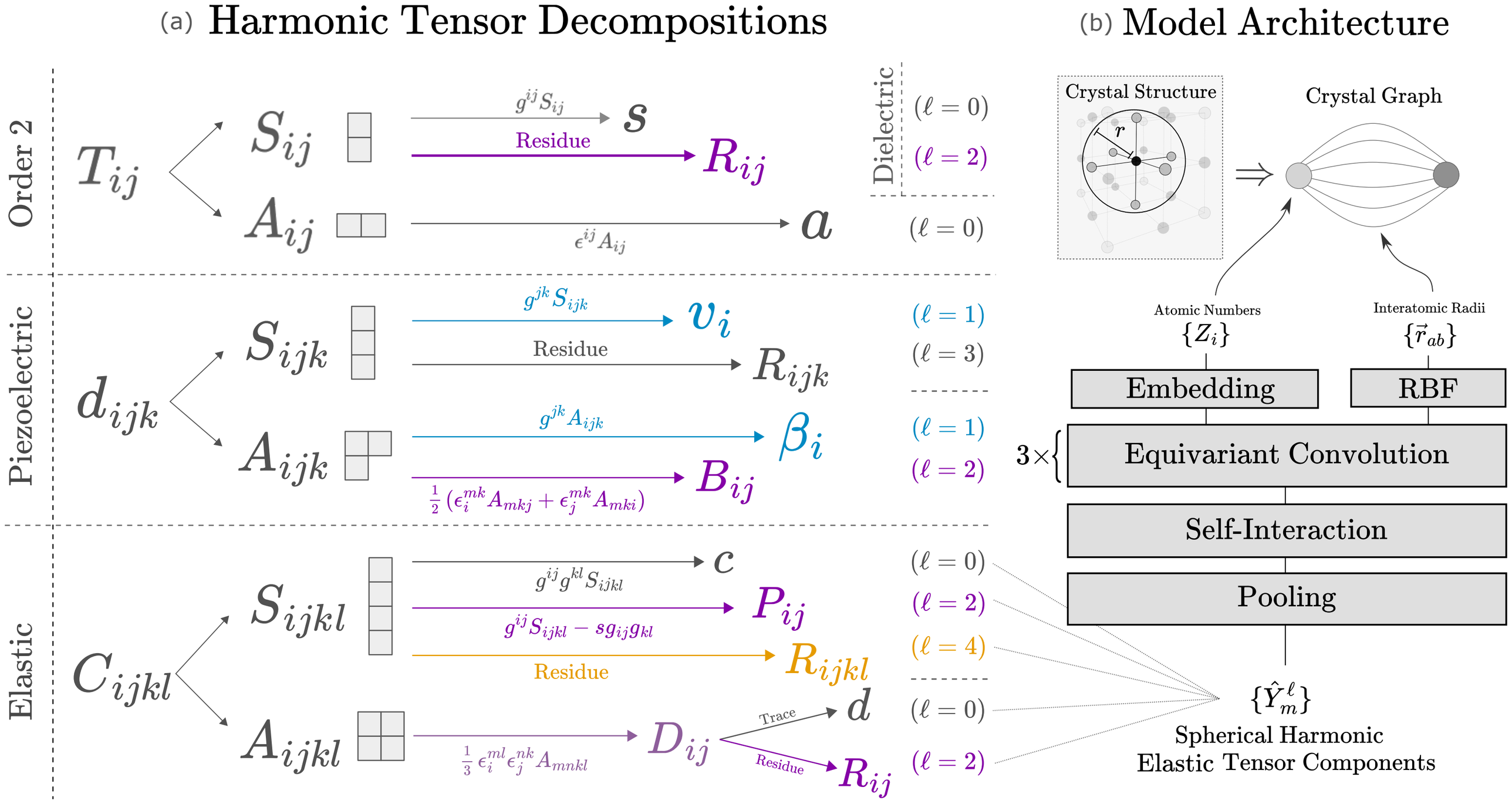
(a) Harmonic Tensor Decompositions
(b) Model Architecture
Order 2
Piezoelectric
Elastic
Dielectric
T_{ij}
S_{ij}
A_{ij}
$g^{ij}S_{ij}$
s
Residue
R_{ij}
$\epsilon^{ij}A_{ij}$
a
$(\ell=0)$
$(\ell=2)$
$(\ell=0)$
d_{ijk}
S_{ijk}
A_{ijk}
$g^{jk}S_{ijk}$
v_i
Residue
R_{ijk}
$g^{jk}A_{ijk}$
β_i
$\frac{1}{2}(\epsilon_i^{mk}A_{mkj}+\epsilon_j^{mk}A_{mki})$
B_{ij}
$(\ell=1)$
$(\ell=3)$
$(\ell=1)$
$(\ell=2)$
C_{ijkl}
S_{ijkl}
A_{ijkl}
$g^{ij}g^{kl}S_{ijkl}$
c
$g^{ij}S_{ijkl}-sg_{ij}g_{kl}$
P_{ij}
Residue
R_{ijkl}
$\frac{1}{3}\epsilon_i^{ml}\epsilon_j^{nk}A_{mnkl}$
D_{ij}
Trace
d
Residue
R_{ij}
$(\ell=0)$
$(\ell=2)$
$(\ell=4)$
$(\ell=0)$
$(\ell=2)$
Crystal Structure
r
Crystal Graph
Atomic Numbers
$\{Z_i\}$
Interatomic Radii
$\{\vec{r}_{ab}\}$
Embedding
RBF
$3\times$
Equivariant Convolution
Self-Interaction
Pooling
$\{\hat{Y}_m^\ell\}$
Spherical Harmonic
Elastic Tensor Components