

Equivariant Tensor Property Prediction with Graph Neural Networks

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Crystal Graph Construction

The usual technique is to represent crystalline systems as graphs (nodes and edges) [1]:



with atomic features associated with nodes and geometric features associated with edges

Message Passing on Graphs

Now, we need to update these features through some trainable function that acts on graph representations.

This is most generally accomplished by a message passing network [2] applied to graph representations.

$$m_i^{t+1} = \sum_{n_j \in \mathcal{N}(i)} M_t(n_i^t, e_{ij}, n_j^t)$$

$$n_i^{t+1} = U_t(n_i^t, m_i^{t+1})$$

Here, each node n from layer t to $t+1$ is updated according to an update function U , which takes as input messages formed from each pair of nodes containing the node to be updated.

Equivariance

A function $f : \mathcal{X} \rightarrow \mathcal{Y}$ between vector spaces is considered equivariant with respect to some group G if for all elements $g \in G$ the following diagram commutes:

$$\begin{array}{ccc} \mathcal{X} & \xrightarrow{f} & \mathcal{Y} \\ D^{\mathcal{X}}(R) \downarrow & & \downarrow D^{\mathcal{Y}}(R) \\ R\mathcal{X} & \xrightarrow{f} & R\mathcal{Y} \end{array}$$

for linear representations D acting on the function's domain and codomain.

SO(3) Equivariant Networks

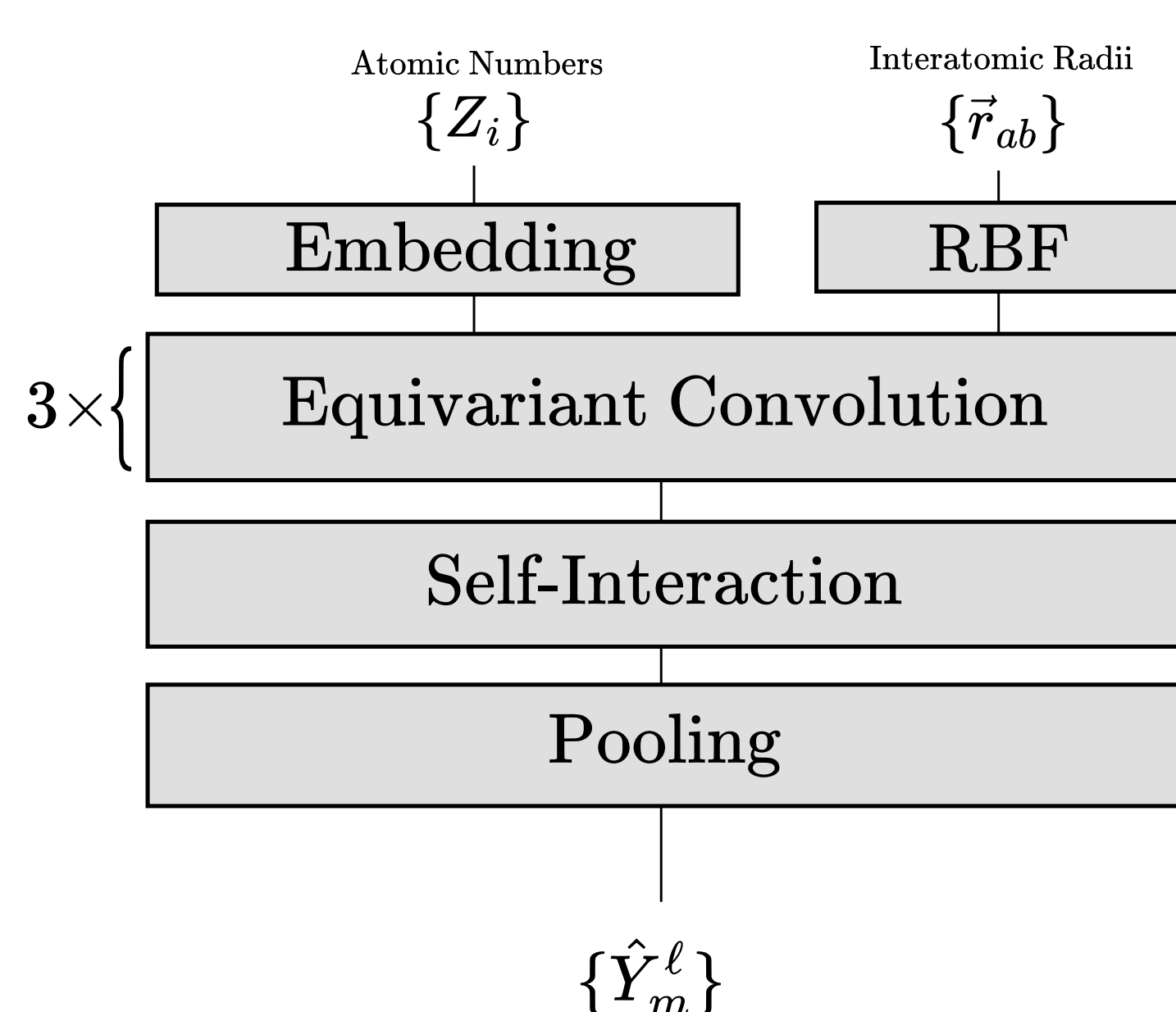
An $SO(3)$ equivariant network is a neural network satisfying:

$$f(\{\mathcal{D}^{\ell_1}(R)h_{(\ell_1)}\}) = \{\mathcal{D}^{\ell_2}(R)h'_{(\ell_2)}\} \quad \forall R \in SO(3)$$

This can be accomplished by associating hidden features V and filters F with spherical harmonics defining convolution as their tensor product [3]:

$$\mathcal{L}_{acm_o}^{\ell_o}(\vec{r}_a, V_{acm_i}^{\ell_i}) = \sum_{m_f, m_i} c_{\ell_i m_i \ell_f m_f}^{\ell_o m_o} \sum_b F_{cm_f}^{\ell_f \ell_i}(r_{ab}) V_{bcm_i}^{\ell_i}$$

Model Architecture [4]



The important thing to note here is that these networks naturally yield coefficients of spherical harmonic tensors.

Clebsch-Gordon Expansion

Build larger spherical harmonic tensors with CG expansion:

$$Y_{\ell_1}^{m_1} \otimes Y_{\ell_2}^{m_2} = \sum_{L=|\ell_1-\ell_2|}^{\ell_1+\ell_2} \sum_{M=-L}^L c_{\ell_1 0 \ell_2 0}^{L 0} c_{\ell_1 m_1 \ell_2 m_2}^{L M} Y_L^M$$

where Y_L represents a $2L+1$ dimensional symmetric tensor space of rank L .

We use this as a relation between symmetric tensor's J_z basis components and higher order spherical harmonic tensors.

$$T^{(n)} = a_{\underbrace{\alpha\beta\ldots}_n} (Y_1^\alpha \otimes Y_1^\beta \otimes \ldots) \Rightarrow y_\ell^m Y_L^M$$

But, what about asymmetric tensors?

SO(3) Invariant Tensor Subspaces

We can always reduce an arbitrary tensor T that transforms under a transformation as:

$$T_{x_1 x_2 \dots x_n} \rightarrow T_{x'_1 x'_2 \dots x'_n} = R_{x'_1}^{x_1} R_{x'_2}^{x_2} \dots R_{x'_n}^{x_n} T_{x_1 x_2 \dots x_n},$$

into a set of irreducible (but not necessarily unique) symmetric, $SO(3)$ invariant subtensors:

$$\{h^{(\ell)}\} \rightarrow \{h'^{(\ell)}\} = \{\mathcal{D}^\ell(R)h^{(\ell)}\}$$

This decomposition can be constructed by consecutive decomposition with respect to GL and then O and SL

$$SO = SL \cap O \subset GL$$

GL Decomposition

- Decompositions under general linear group GL are simultaneous with decompositions under symmetric group S (*Schur-Weyl Duality*)
- Irreducible representations of symmetric group are diagrammatically described by Young diagrams.

O Decomposition

Young diagrams are said to be of some shape $\lambda : (\lambda_1, \lambda_2, \dots, \lambda_k)$, where λ_i refers to the depth of row i and $\lambda_{i+1} \leq \lambda_i \leq \lambda_{i-1}$. Above: (5, 4, 3, 1)

Orthogonal group O , preserves inner product between vectors $\langle \cdot, \cdot \rangle$. defined by means of a metric tensor g_{ij} , which transforms as a second rank tensor under some transformation R as:

$$g_{x_1 x_2} \rightarrow g_{x'_1 x'_2} = R_{x'_1}^{x_1} R_{x'_2}^{x_2} g_{x_1 x_2}$$

Contractions of arbitrary tensors T with g_{ij} are invariant under O .

SL Decomposition

Special linear group SL of transformations is defined as invertible linear transformations with determinant equal to positive one.

Under SL , orientation and volume are preserved, where volume is defined as the contraction of a tensor with the fully antisymmetric tensor ϵ_{ijk} , which transforms under $R \in GL(3)$ as:

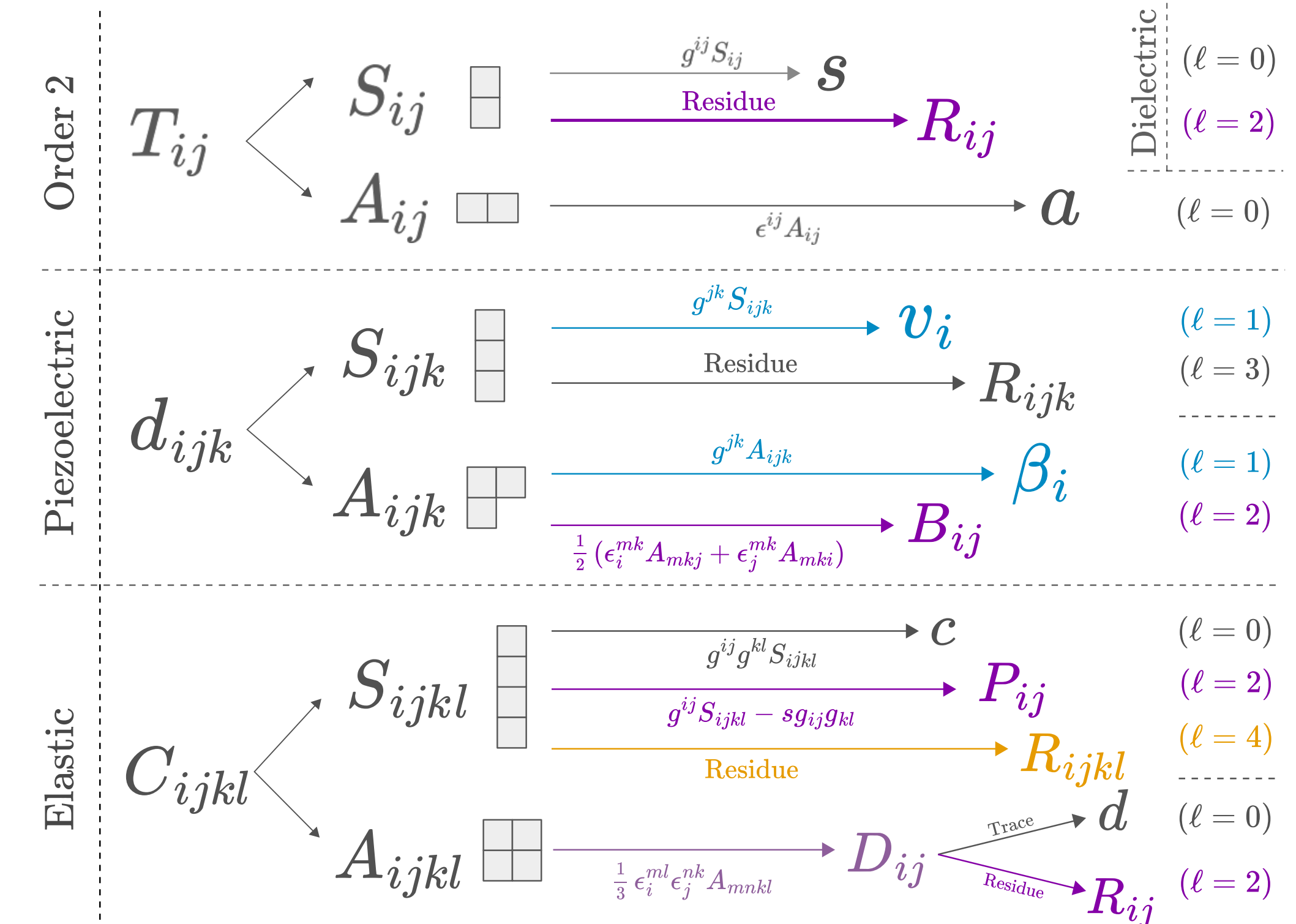
$$\epsilon_{x_1 x_2 x_3} \rightarrow \epsilon_{x'_1 x'_2 x'_3} = \det(R) R_{x'_1}^{x_1} R_{x'_2}^{x_2} R_{x'_3}^{x_3} \epsilon_{x_1 x_2 x_3}$$

Similar to the case of g_{ij} in O , contractions with ϵ_{ijk} of arbitrary tensors yield SL invariant subspaces.

Materials Project Database

The Materials Project [5] provides calculated scalar and tensorial properties for a large set of 150,000 materials. After pruning, we are left with 7,273 dielectric tensors, 3,292 piezoelectric tensors, and 10,286 elastic tensors.

Tensor Decompositions



Dielectric Tensor

The dielectric permittivity tensor ϵ of some material is a linear model of it's electric displacement \vec{D} in response to an external electric field \vec{E} :

$$\vec{D} = \epsilon \vec{E}$$

Piezoelectric Tensor

The piezoelectric strain constants $(d_{ijk})_T$ are defined by:

$$(d_{ijk})_T = \left(\frac{\partial \epsilon_{ij}}{\partial E_k} \right)_{\sigma, T}$$

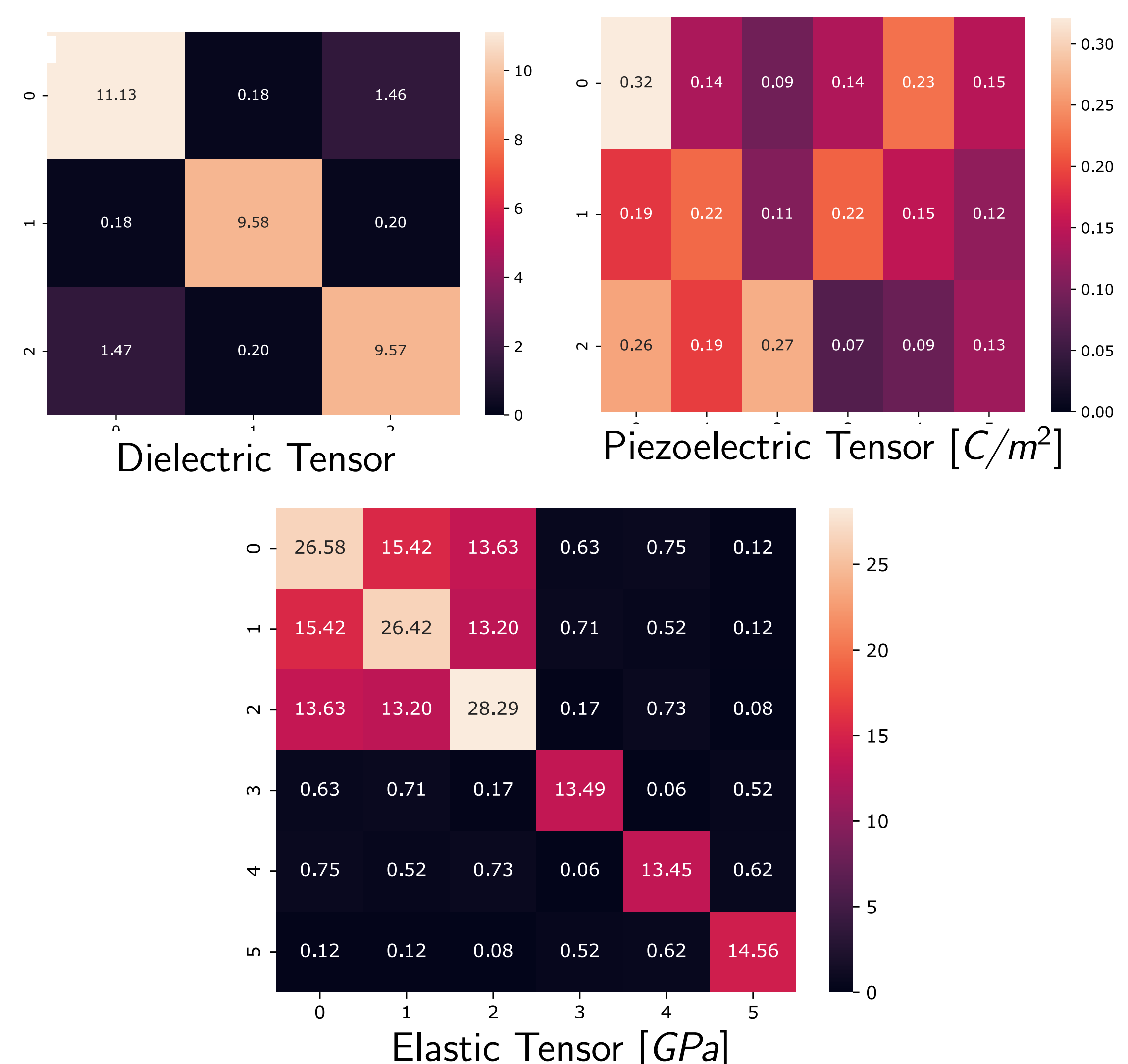
where here ϵ is the strain tensor, and the partial derivative is taken at constant stress σ and temperature T .

Elastic Tensors

The elasticity (or simply, elastic) tensor C of a material relates it's Cauchy strain ϵ to some infinitesimal stress τ . This may be described, component-wise, as the linear relation below:

$$\tau_{ij} = C_{ijkl} \epsilon_{kl}$$

Prediction Results



References

- [1] Phys. Rev. Lett. **120**, 145301 (2018)
- [2] <https://arxiv.org/abs/1704.01212>
- [3] <https://arxiv.org/abs/1802.08219>
- [4] <https://arxiv.org/abs/2406.03563>
- [5] <https://materialsproject.org/>