DeepSciReasoner

Deep Scientific Reasoning under Physical Constraints: Structure-Aware Spectrum Prediction

Yingheng Wang[1], Tao Yu[2], Francesco Ricci[3,4],
Shufeng Kong[1,2], John M. Gregoire[5,6], Carla P. Gomes[1]

Cornell University,
Sun Yat-sen University, UCLouvain, Matgenix SRL, CalTech, Lila Sciences

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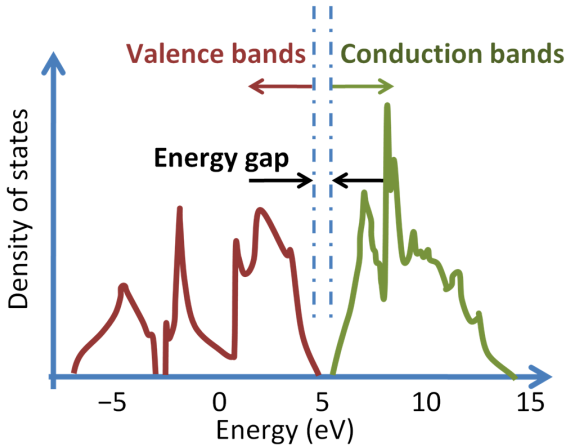
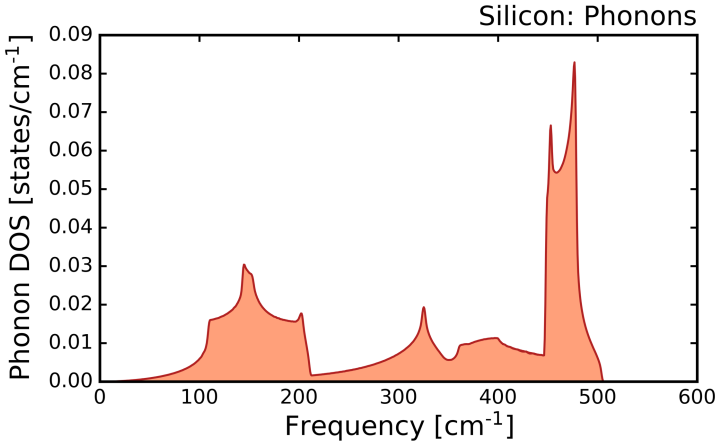
Spectrum properties are ubiquitous across molecular systems!

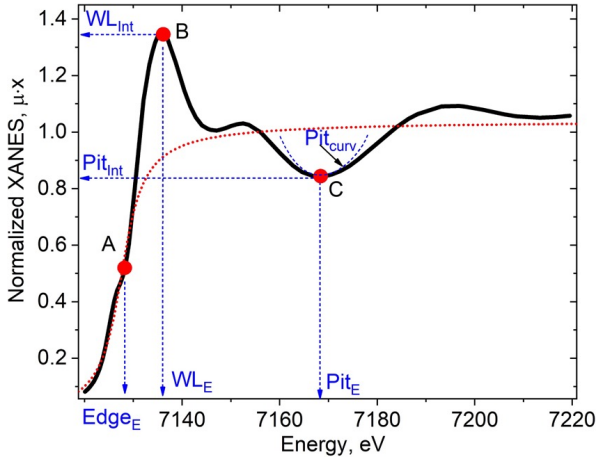
Electronic Density of States (eDOS)



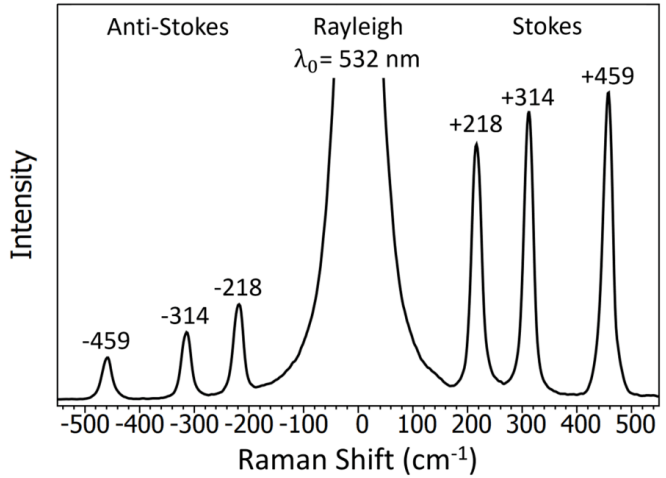
Phonon Density of States (phDOS)



X-ray Absorption Near-Edge Structure (XANES)



Raman Spectra



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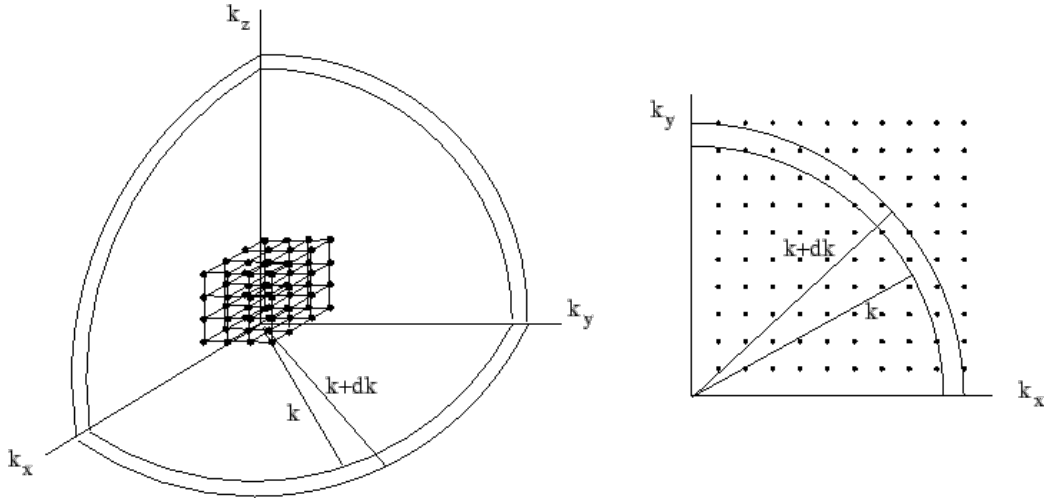
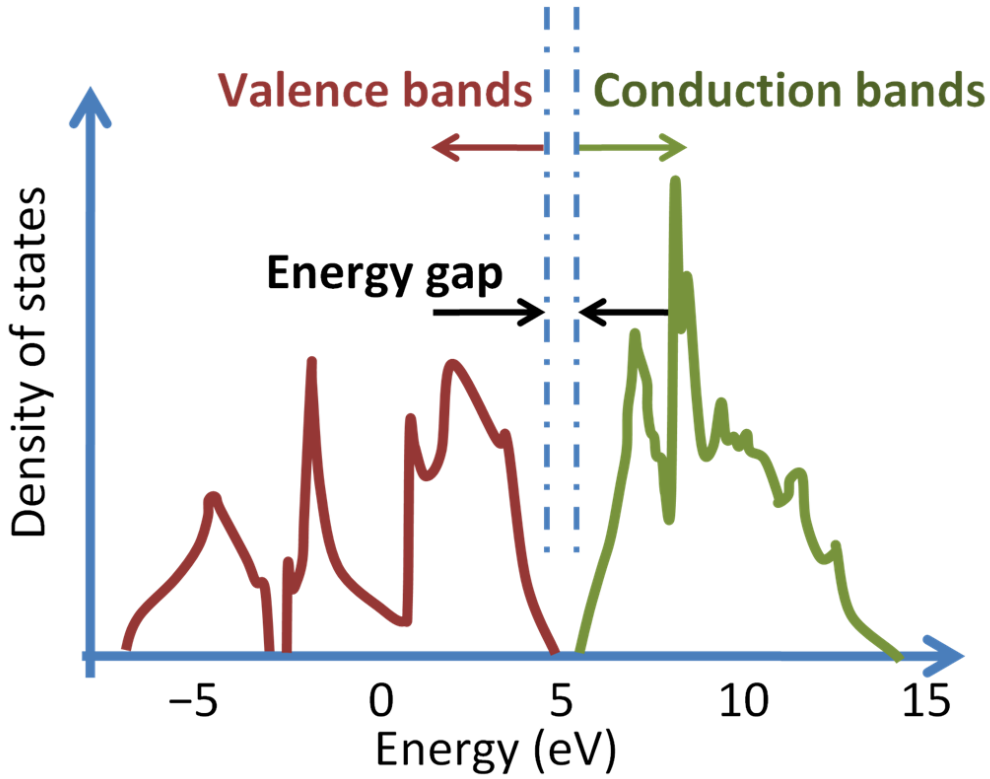
eDOS: how many "slots" are available for electrons at a given energy.

$$D(E) = \frac{\mathrm{d}N(E)}{\mathrm{d}E}$$



Determines a material's ***electrical***, ***optical***, ***magnetic***, and ***catalytic*** properties.



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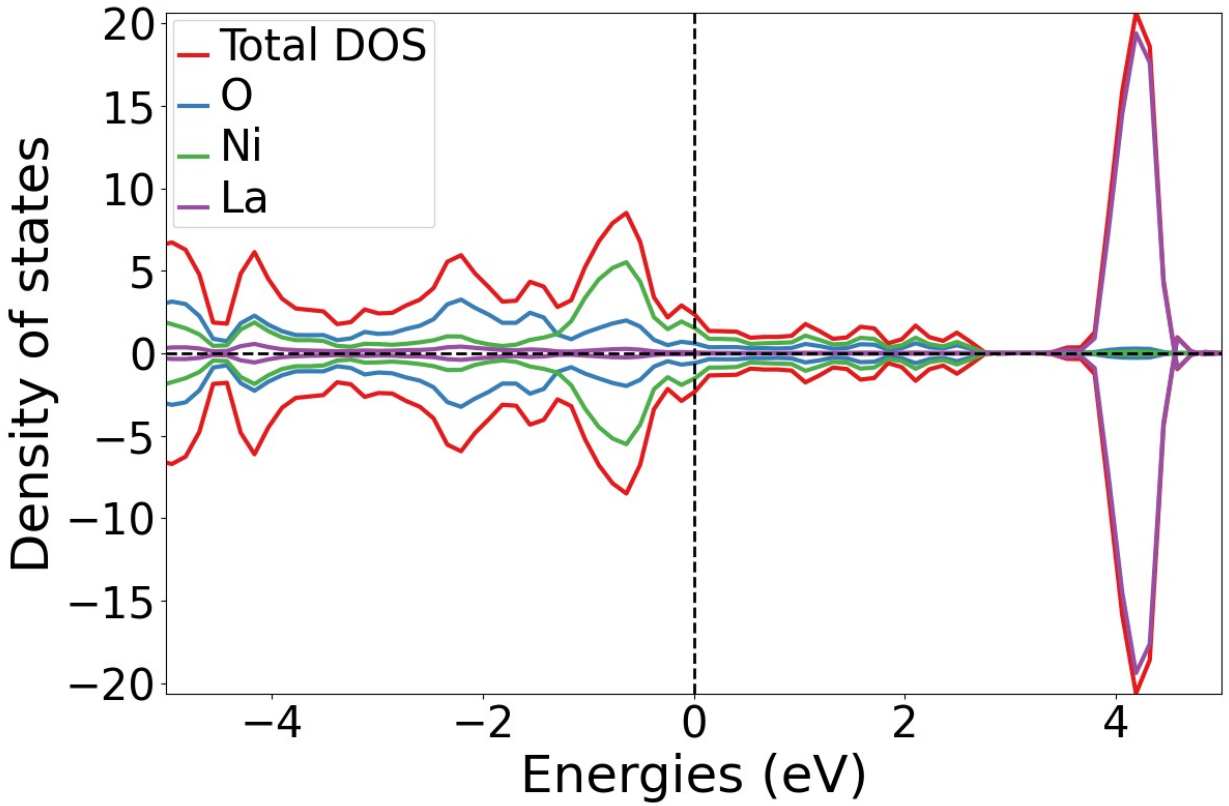
eDOS: include total DOS and partial DOS (pDOS)

(1) elemental projections (2) atomic projections



Labels missing or even unavailable!

Capture it in an unsupervised way

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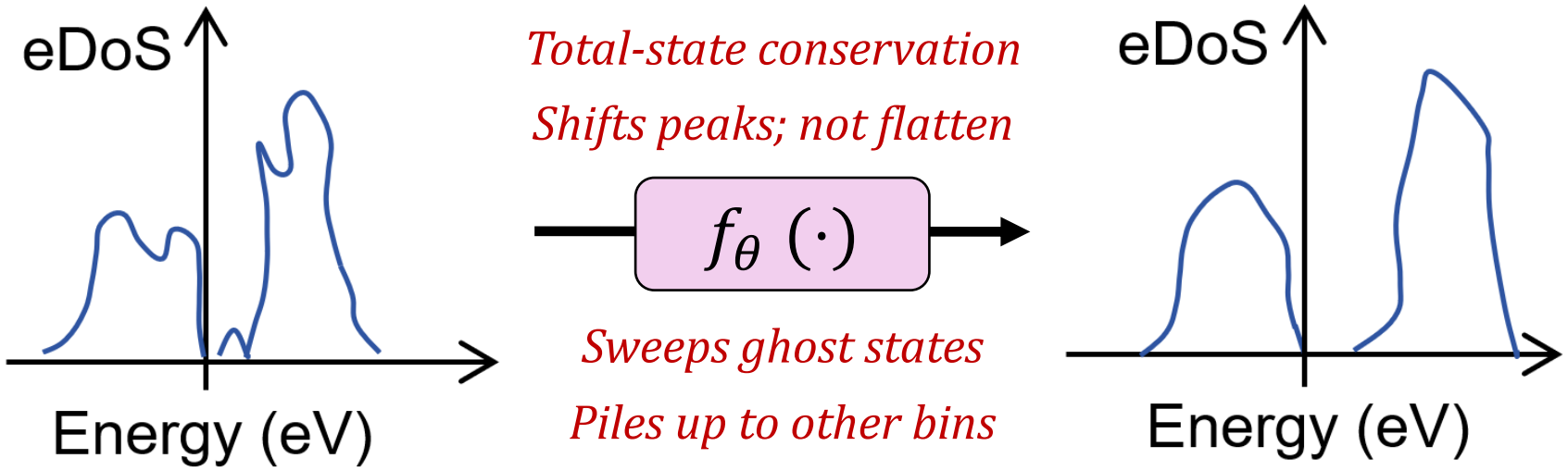
Black-box predictor violates physics:

- (1) noise ("ghost states") in band gap
- (2) post-hoc correction violates total-state conservation
- (3) smeared/flattened to minimize MSE/MAE



Coarse Prediction

Ground Truth

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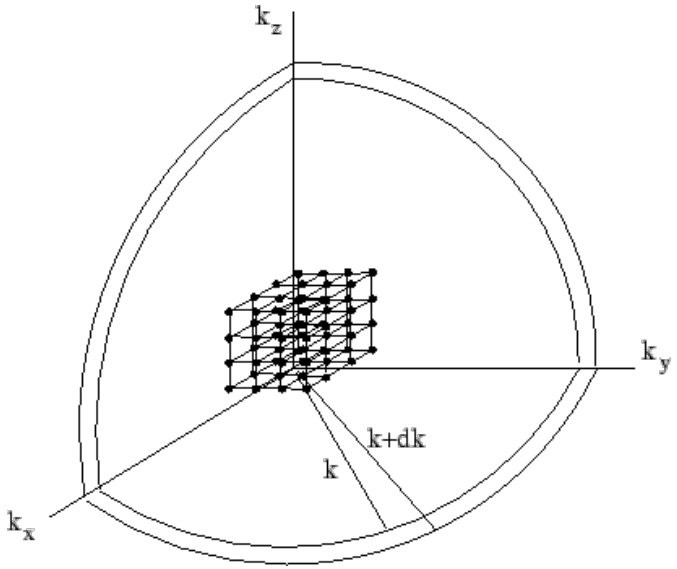

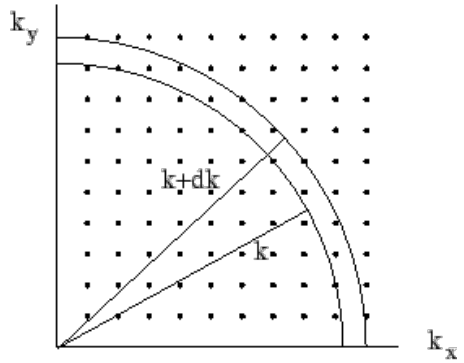

Electronic DOS: very hard to compute in practice

$$g(E) = \sum_n \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\, \delta(E - E_n(\mathbf{k}))$$

exp. in # electrons

Schrödinger Equation

$$\left[\underbrace{-\sum_{i=1}^{N} \frac{\hbar^2}{2m_e}\nabla_i^2}_{\text{(1) Electron kinetic energy}} + \underbrace{\frac{1}{2}\sum_{i\neq j}^{N} \frac{e^2}{4\pi\epsilon_0 |r_i - r_j|}}_{\text{(2) Electron–electron repulsion}} - \underbrace{\sum_{i=1}^{N}\sum_{\alpha=1}^{K} \frac{e^2 Z_\alpha}{4\pi\epsilon_0 |r_i - R_\alpha|}}_{\text{(3) Electron–nucleus attraction}} \right] \Psi = E\Psi$$

Density Functional Theory

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{eff}}[n(\mathbf{r})] \right] \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r})$$

Very slow; days to weeks for systems containing hundreds of atoms

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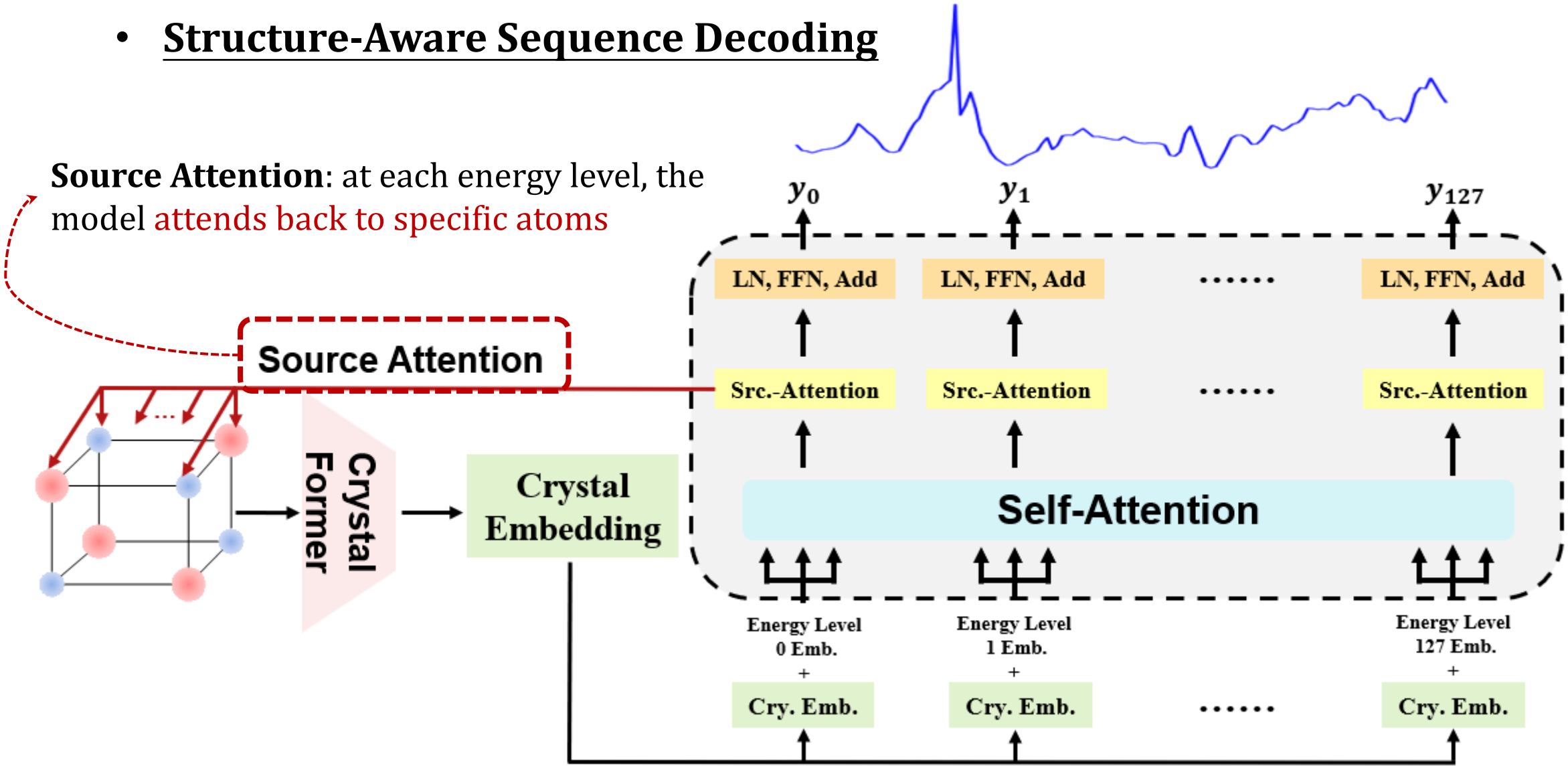
- **Structure-Aware Sequence Decoding**

Source Attention: at each energy level, the model attends back to specific atoms



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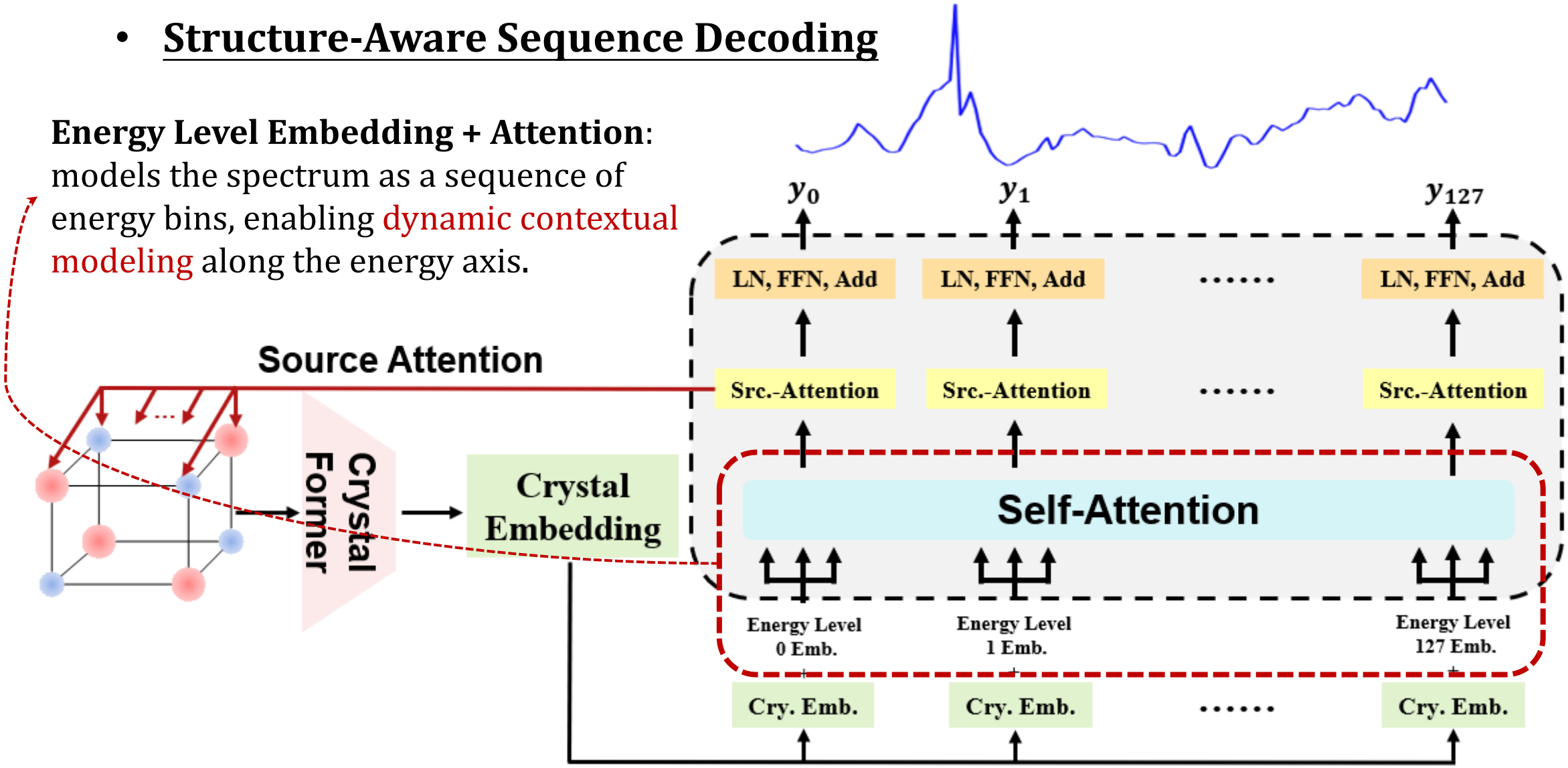
- **Structure-Aware Sequence Decoding**

Energy Level Embedding + Attention: models the spectrum as a sequence of energy bins, enabling dynamic contextual modeling along the energy axis.



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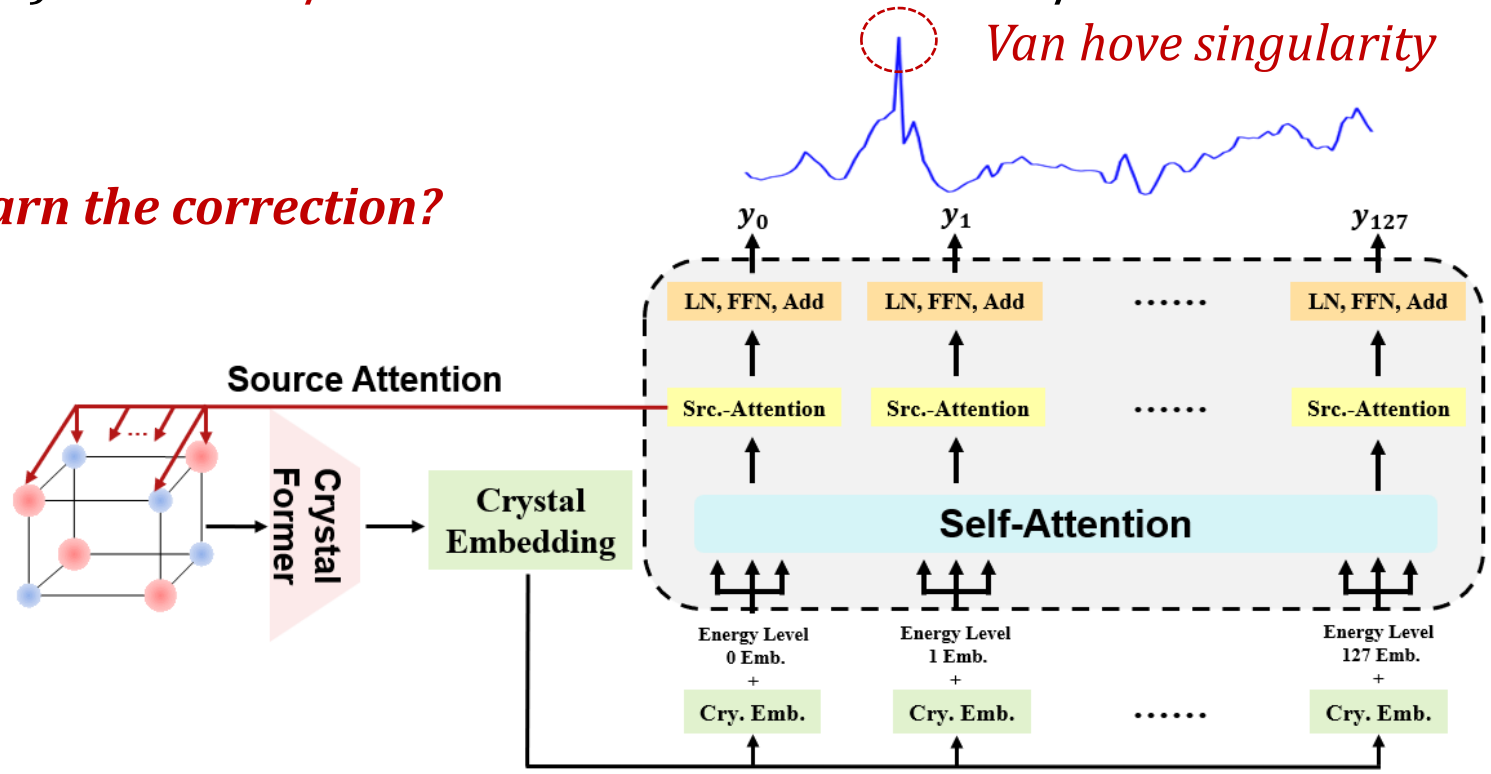
- **Structure-Aware Sequence Decoding**
  - Black-box predictor violates physics:
    - (1) noise ("ghost states") in band gap
    - (2) post-hoc correction violates mass conservation
    - (3) smeared/flattened to minimize MSE/MAE

How can we learn the correction?



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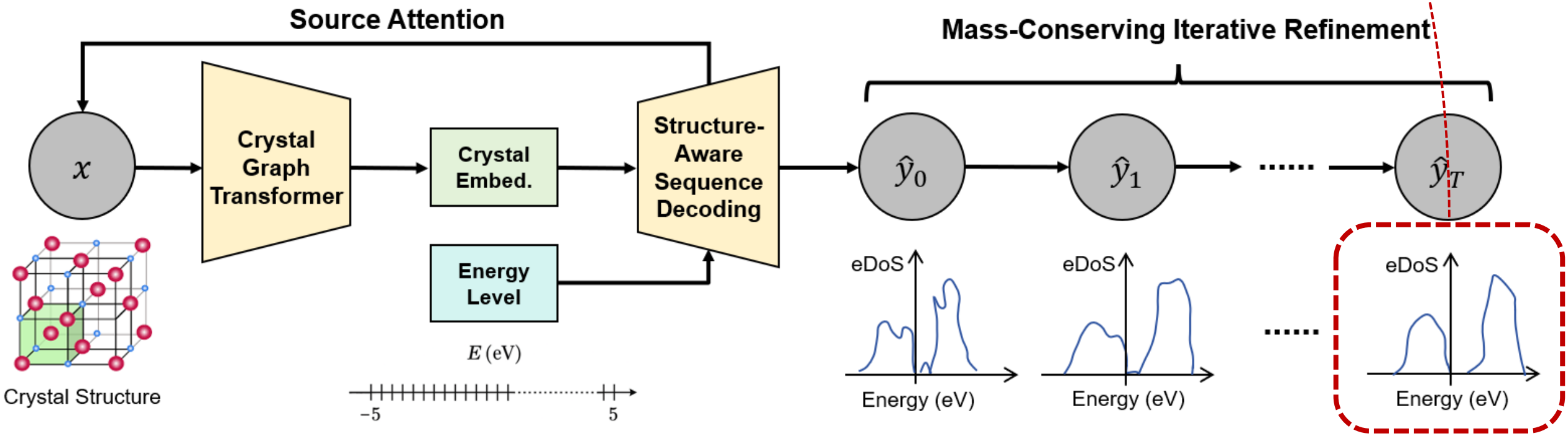
- **Constraint-Preserving Physical Reasoning**
  - Normalized DoS can be viewed as 1D probability density
  - Mass conservation law states that

inflow $\dfrac{d}{dt}\int_{\Omega} p_\theta(x,t)\,dx = -\oint_{\partial\Omega} p_\theta(x,t)\, f_\theta(x,t)\cdot n\, dS$ outflow



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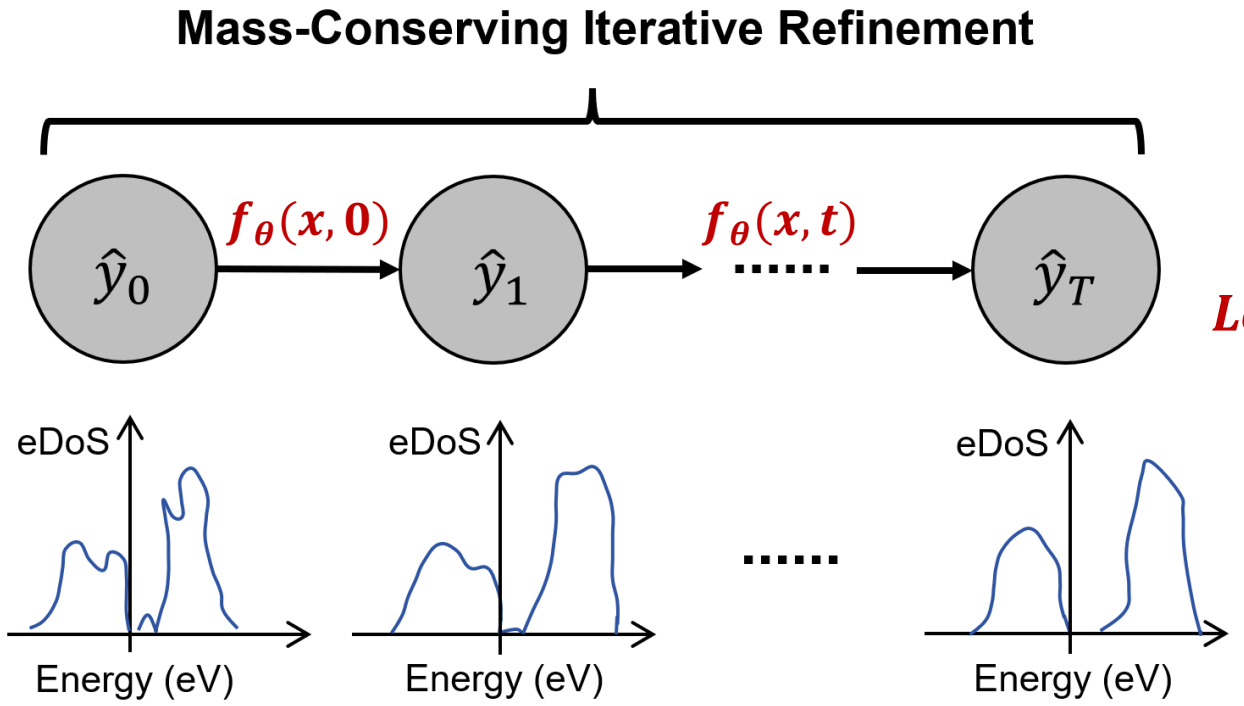
- **Constraint-Preserving Physical Reasoning**
  - Model the temporal evolution of normalized DoS under the continuity equation (*divergence theorem*):

$$\partial_t p(x,t) + \nabla \cdot \left(p(x,t) f_\theta(x,t) \right) = 0$$

Infinite satisfied vector fields!



Learning the probability transport!

Chen, et al. (2018)

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- **Constraint-Preserving Physical Reasoning**
  - Wasserstein-2 distance **[Benamou-Brenier, 2000]:**

$$W_2^2(p_0, p_T) = \inf_{p_t, f_t} \int_0^1 \int p_t(x) \, \| f_t(x) \|^2 \, dx \, dt,$$

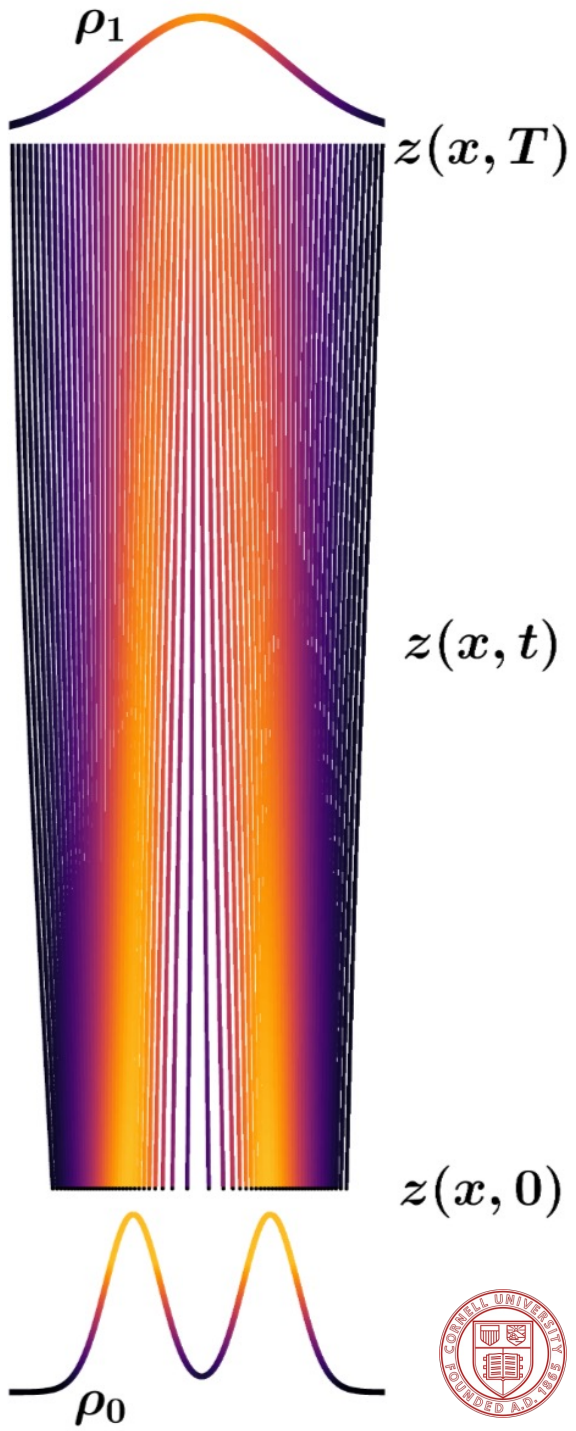
$$\text{s.t.} \quad \partial_t p_t + \nabla \cdot (p_t f_t) = 0$$

  - W2 displacement interpolation (optimal transport map):

$$x_t(s) = (1-t)x_0(s) + t x_T(s), \quad p_t = (x_t)_{\#} p_0$$

  - Reference vector field:

$$f_t(x_t(s)) = x_T(s) - x_0(s)$$



Benamou and Brenier (2000)

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- **Constraint-Preserving Physical Reasoning**

  - Training:

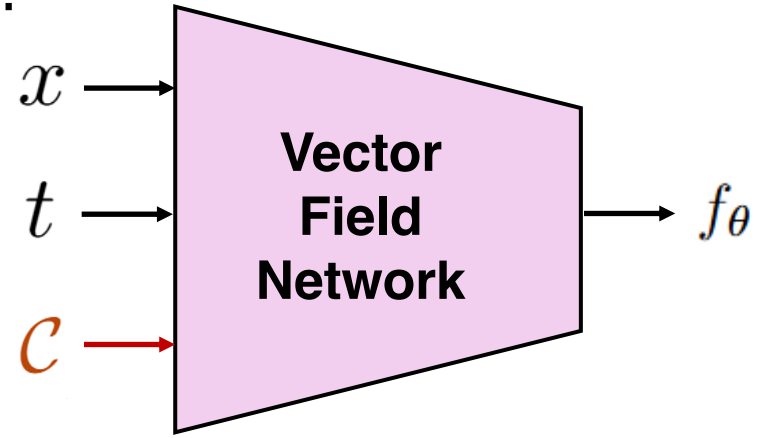
$$\mathcal{L}(\theta) = \mathbb{E}_{(x,t)\sim\mathcal{D}}\left[\|f_\theta(x,t) - f_t(x)\|^2\right]$$

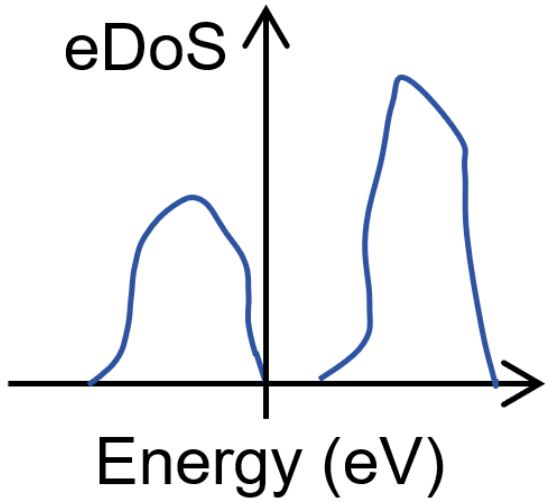
  - Inference:

$$\partial_t F_\theta(x,t) + f_\theta(x,t)\,\partial_x F_\theta(x,t) = 0, \qquad F_\theta(x,0) = F_0(x).$$

$$\hat{p}_T(x) := p_\theta(x,T) = \partial_x F_\theta(x,T)$$

  - Amortized inference:



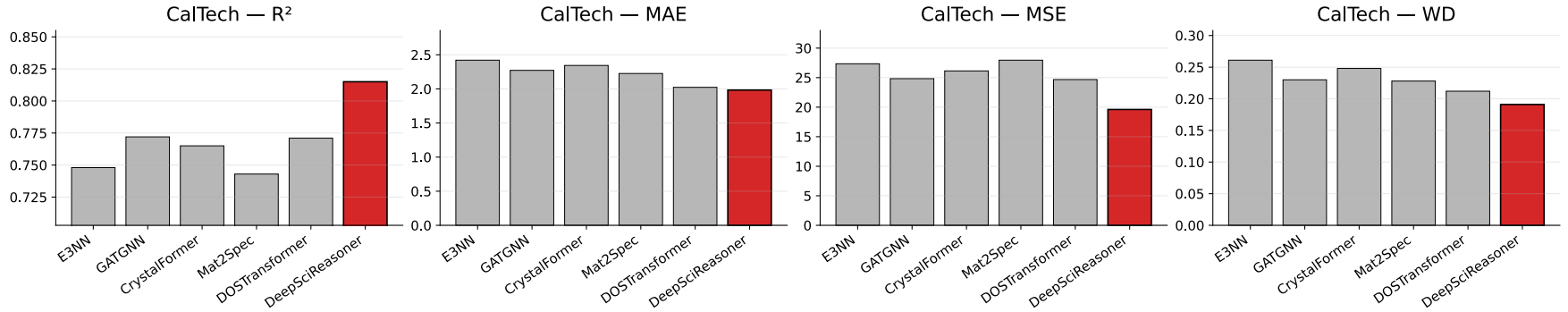


Song et al. (2020); Lipman, et al. (2022)

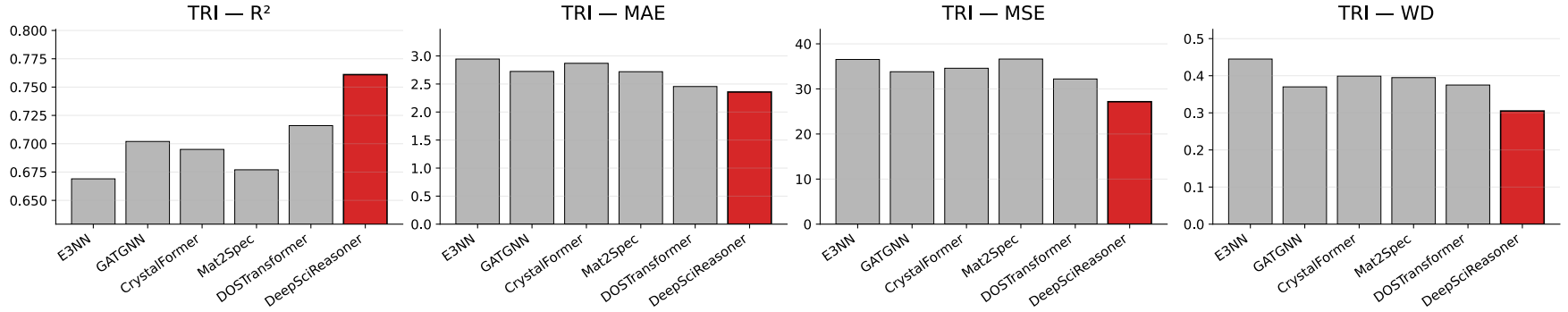
Experimental Results: eDOS prediction

Method	CalTech				TRI			
	$R^2\uparrow$	MAE$\downarrow$	MSE$\downarrow$	WD$\downarrow$	$R^2\uparrow$	MAE$\downarrow$	MSE$\downarrow$	WD$\downarrow$
E3NN	0.748±0.002	2.421±0.003	27.351±0.629	0.261±0.005	0.669±0.004	2.945±0.005	36.535±0.532	0.445±0.004
GATGNN	0.772±0.001	2.272±0.016	24.831±0.585	0.230±0.004	0.702±0.004	2.724±0.004	33.811±0.420	0.370±0.003
CrystalFormer	0.765±0.006	2.344±0.016	26.138±0.477	0.248±0.012	0.695±0.010	2.869±0.082	34.584±0.581	0.399±0.017
Mat2Spec	0.743±0.002	2.226±0.010	27.955±0.137	0.228±0.013	0.677±0.002	2.719±0.072	36.628±0.105	0.395±0.009
DOSTransformer	0.771±0.002	2.023±0.032	24.675±0.354	0.212±0.040	0.716±0.003	2.455±0.080	32.208±0.288	0.375±0.014
DeepSciReasoner	**0.815**±0.007	**1.983**±0.021	**19.612**±0.225	**0.191**±0.017	**0.761**±0.009	**2.357**±0.046	**27.162**±0.563	**0.305**±0.011

CalTech



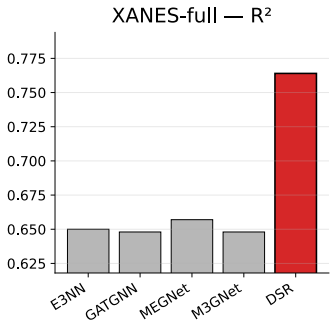
TRI

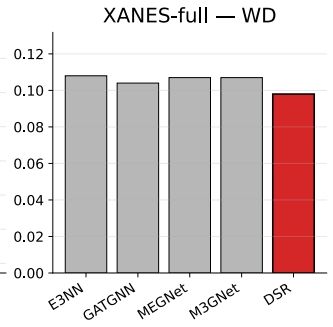


Experimental Results: XANES, Raman, & phDOS

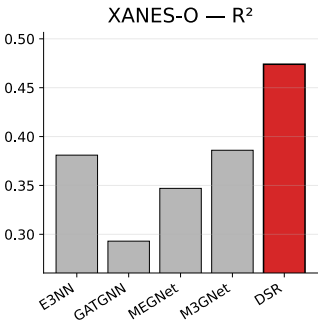
Method	XANES-full		XANES-O		Raman		phDOS			
	$R^2\uparrow$	WD$\downarrow$	$R^2\uparrow$	WD$\downarrow$	$R^2\uparrow$	WD$\downarrow$	$R^2\uparrow$	MAE$\downarrow$	MSE$\downarrow$	WD$\downarrow$
E3NN	0.650±0.012	0.108±0.003	0.381±0.011	0.099±0.004	0.096±0.005	0.451±0.019	0.506±0.015	0.082±0.003	0.026±0.001	0.103±0.004
GATGNN	0.648±0.005	0.104±0.001	0.293±0.013	0.108±0.002	0.115±0.005	0.526±0.008	0.270±0.025	0.106±0.002	0.038±0.003	0.155±0.008
MEGNet	0.657±0.008	0.107±0.002	0.347±0.020	0.102±0.006	0.045±0.004	0.449±0.024	0.538±0.014	0.080±0.003	0.024±0.001	0.094±0.004
M3GNet	0.648±0.010	0.107±0.002	0.386±0.012	0.096±0.005	0.083±0.003	0.426±0.021	0.543±0.012	0.075±0.003	0.023±0.001	0.075±0.003
DSR	**0.764**±0.009	**0.098**±0.003	**0.474**±0.010	**0.093**±0.003	**0.264**±0.002	**0.423**±0.017	**0.636**±0.013	**0.062**±0.004	**0.021**±0.002	**0.061**±0.002

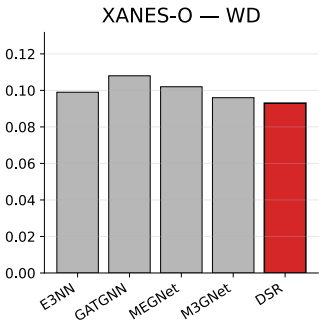
XANES-full



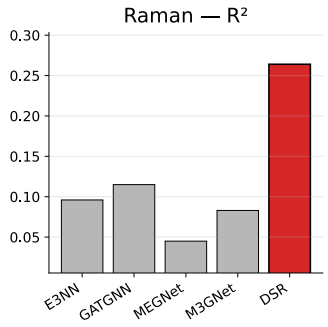


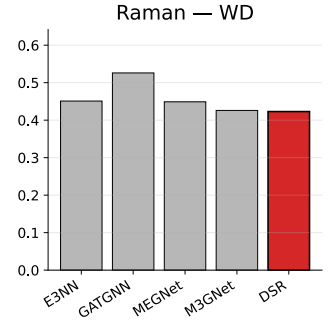
XANES-O



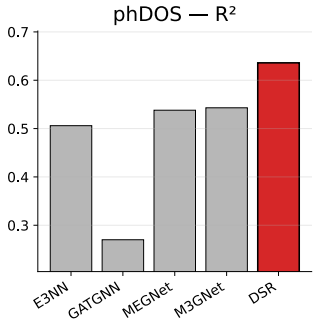


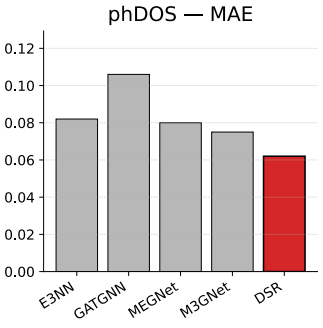
Raman

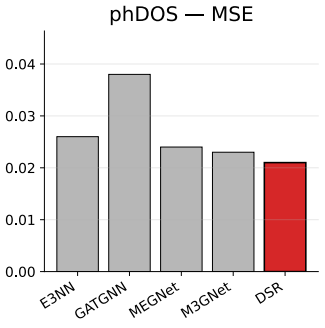


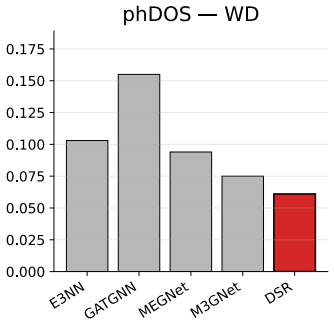


phDOS





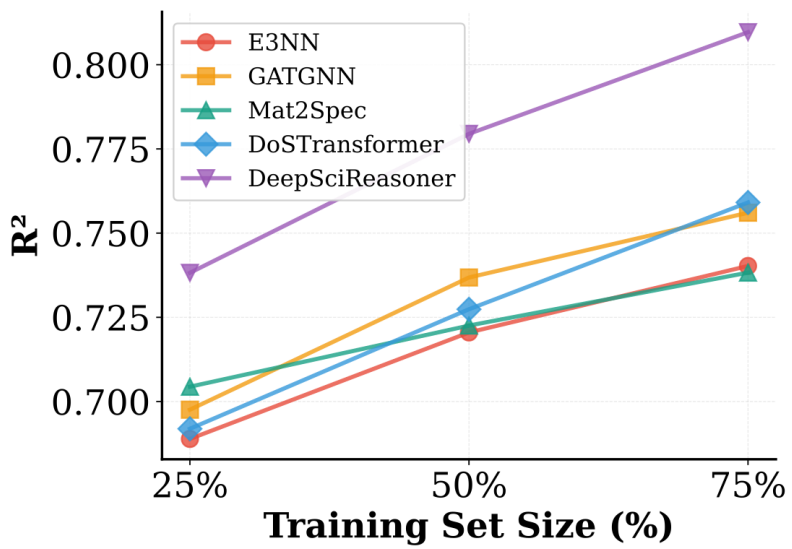


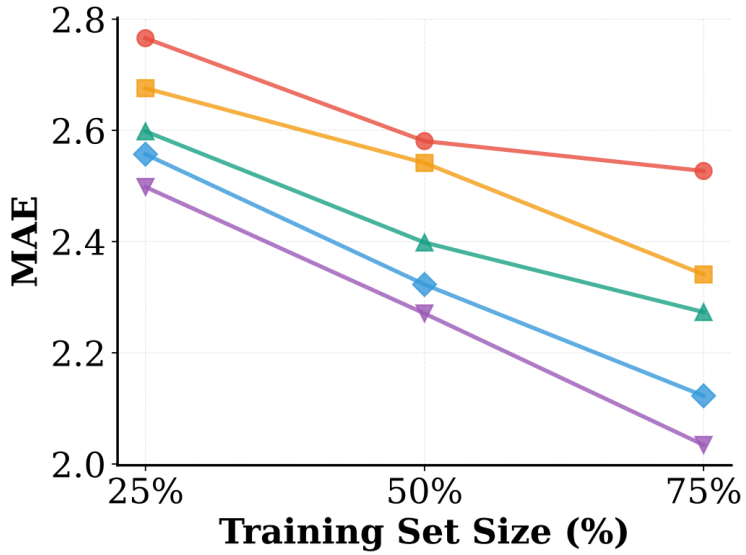


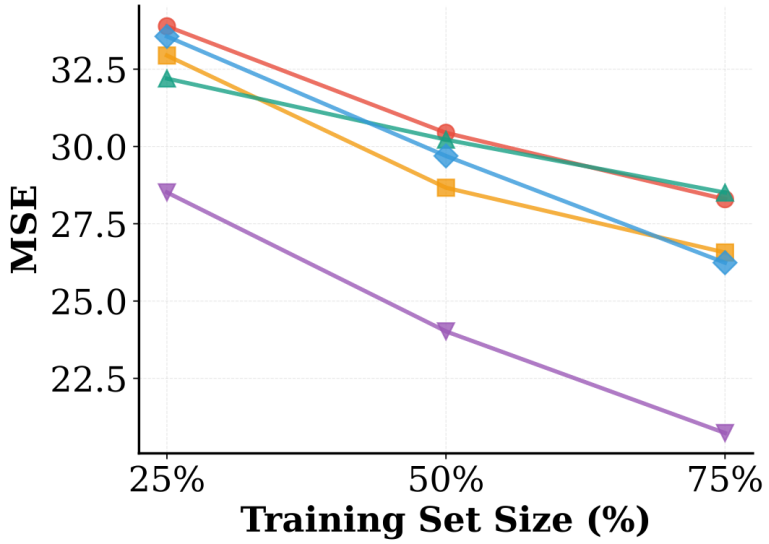
Experimental Results: data scaling

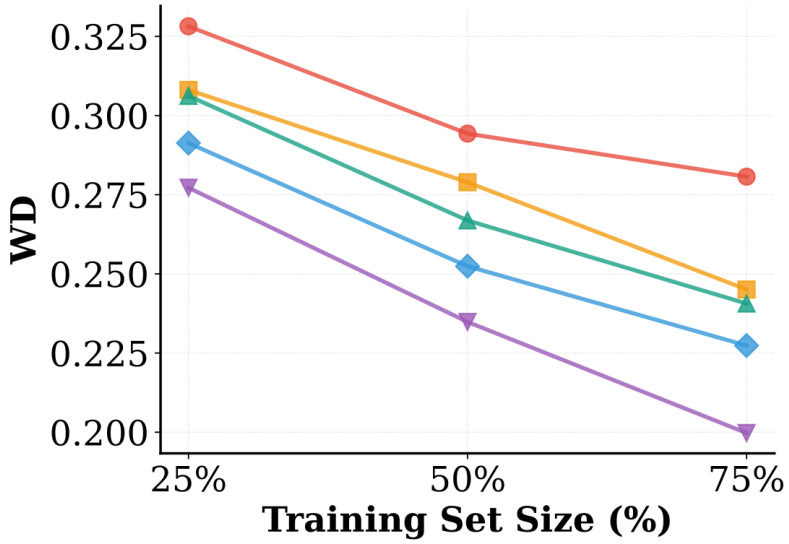
Sample efficient!

Achieve the same performance using only 25% training data

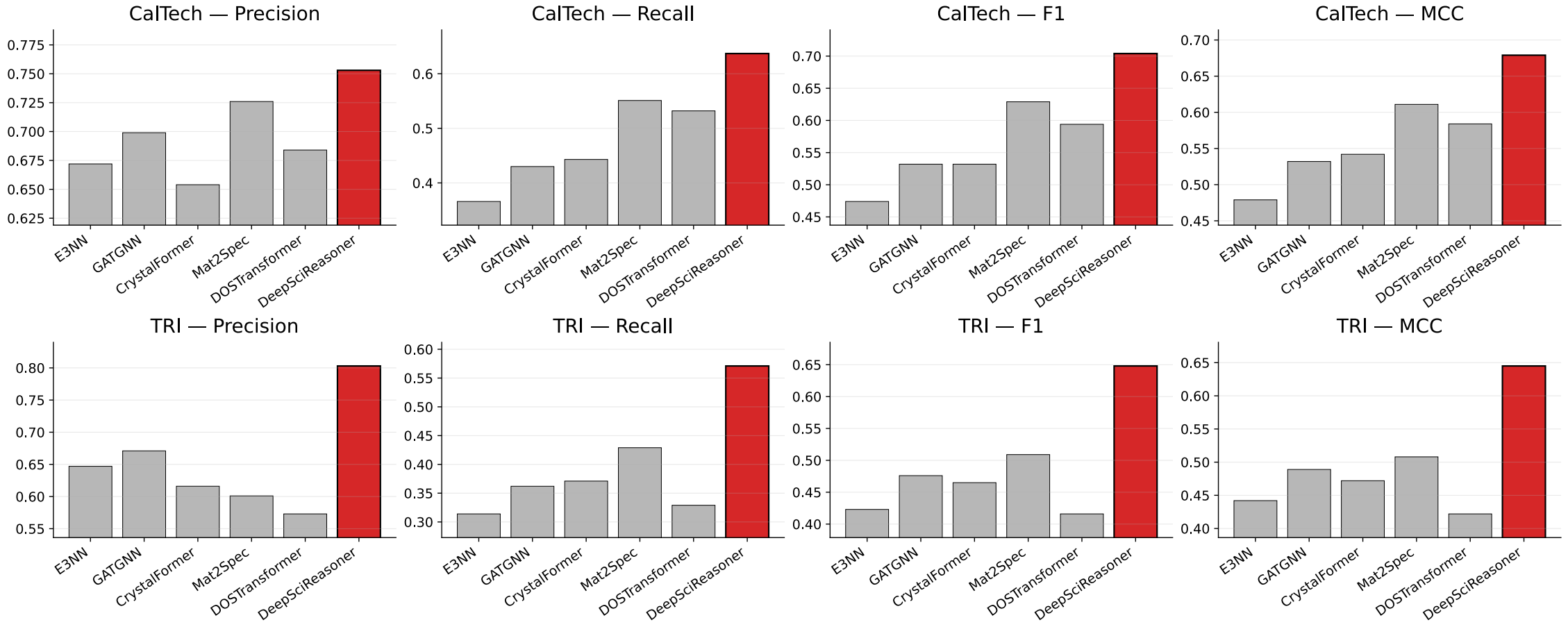






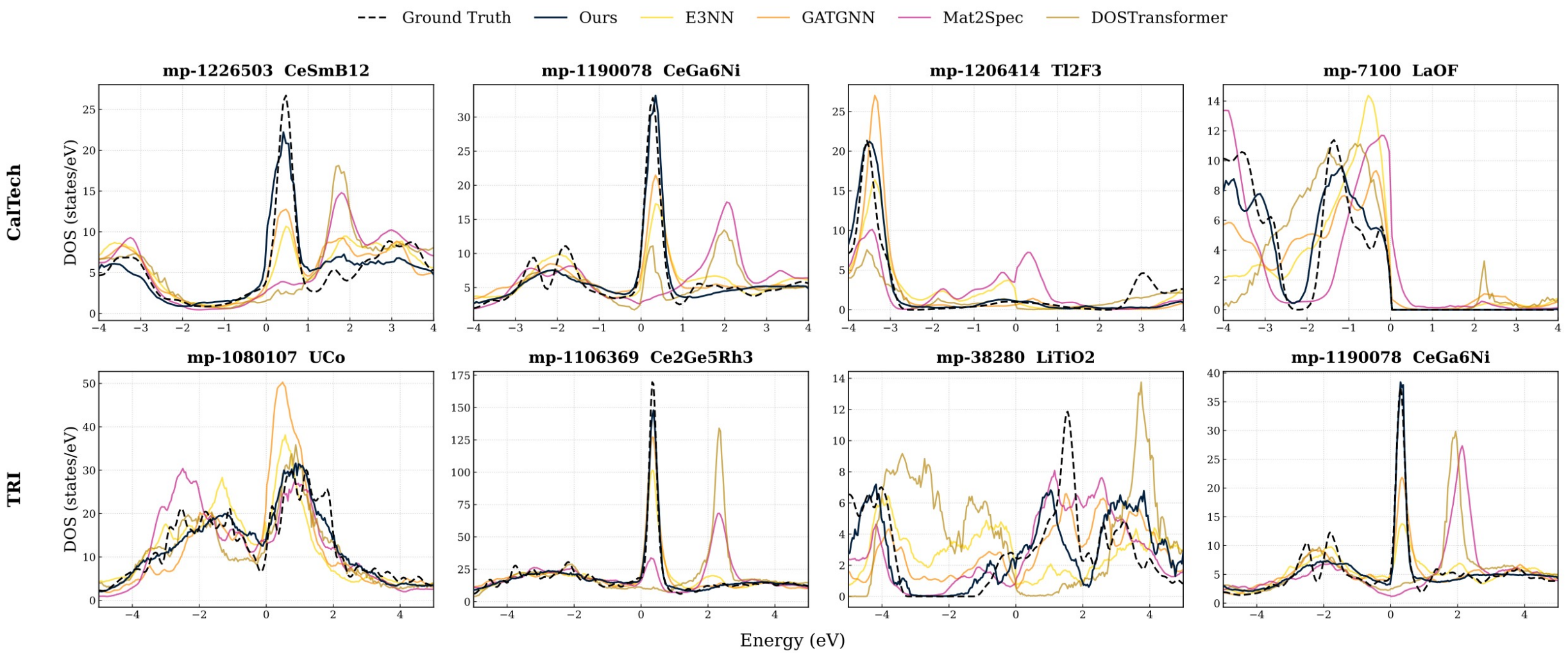


Experimental Results: VB-gap identification



Better identify the sharp edges and gaps in valence band of eDOS!

Experimental Results: visualization



Match peaks, sharp edges and gaps better!

Thank you!

Check our paper for more details.