OptiXNet: Symmetry-Aware Equivariant Network for Discovering SHG-Active Materials

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The search for materials with strong second-harmonic generation (SHG) remains a central challenge in modern photonics, as such materials are critical for frequency conversion, optical communication, and solid-state laser technologies. Efficient nonlinear optical crystals enable wavelength conversion across ultraviolet, visible, and infrared regimes, but identifying compounds that simultaneously exhibit large SHG response, wide band gaps, and suitable birefringence remains difficult. Traditional first-principles methods such as density functional theory provide accurate predictions but are computationally expensive, limiting their use in large-scale exploration of chemical space.

Despite rapid progress in machine learning for materials science, most existing models are restricted to predicting scalar descriptors or simplified SHG metrics [1,2]. Direct prediction of the full SHG tensor is significantly more challenging, as it is an orientation-dependent tensorial property governed by crystal symmetry. In this talk, we introduce OptiXNet (Figure 1), a symmetry-aware equivariant graph neural network designed to predict the complete SHG tensor while strictly preserving physical and symmetry constraints [3]. Trained on the NOEMD database, OptiXNet achieves a test RMSE of 0.141 for the maximum SHG tensor component, substantially outperforming baseline models such as ALIGNN (test RMSE of 0.24). The model also demonstrates consistent accuracy across all tensor elements and reliable generalization across diverse chemical compositions. At the moment, that is the only ML model which can predict complete SHG tensor with high accuracy.

Using the trained model, we performed large-scale screening of non-centrosymmetric materials from crystallographic databases and evolutionary structure searches. OptiXNet successfully rediscovered well-known nonlinear optical crystals, which were not presented in the training set, including $Li_2Si_2O_5$, $Zn(PO_3)_2$, $Ca_5B_3O_9F$, and $CsZnPO_4$, while also identifying nearly one hundred previously unexplored candidate materials. In particular, a new fluorophosphate system, $MgP_2O_5F_2$, was predicted to exhibit strong SHG response, with several stable polymorphs showing SHG coefficients around 1.0–1.1×KDP and large band gaps above 7.8 eV. Subsequent density functional theory calculations confirmed the model's predictions. These results demonstrate that symmetry-aware equivariant learning enables accurate, high-throughput prediction of nonlinear optical tensors and provides a powerful route for the accelerated discovery of next-generation SHG-active materials.

References

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Figures

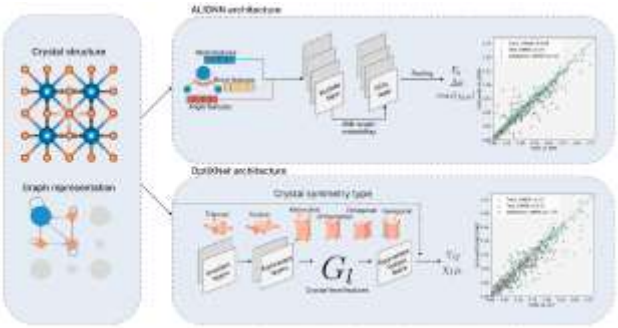

Figure 1. OptiXNet model architecture and performance evaluation on SHG prediction.