PHYSICAL MATH SEMINAR

Though This Be Disorder, Yet There Is Order in't

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ABSTRACT:

Understanding the relationship between structure and properties is crucial to designing materials with novel functions. Crystals have proven to be a highly versatile platform for engineering functions, as the periodicity of their atomic arrangement greatly facilitates the prediction and optimization of their properties. However, not all properties can be realized with periodic structures. Correlated disordered media — materials that do not exhibit conventional forms of long-range order — can achieve transport properties unattainable in periodic systems, such as the formation of isotropic photonic bandgaps, which are highly desirable in optoelectronic applications. By the very nature of disorder, identifying principles and approaches to engineer disordered functional materials is very challenging — in fact, what does it even mean to "engineer disorder"? In this talk, I will show how we established a new state of the art in the design of correlated disordered structures. This approach led us to the discovery of a new class of disordered functional materials that we termed "gyromorphs", which uniquely combine liquidlike translational disorder with quasi-long-range rotational order, induced by a ring of delta peaks in their structure factor. We predict that gyromorphs outperform all existing isotropic photonic bandgap materials, paving the way for fine control over optical properties. Finally, I will provide an outlook and discuss recent results on how we are leveraging noisy processes to build generative AI models that will accelerate the discovery of novel materials across the periodic table. "Though this be madness, yet there is method in't" (Hamlet II.ii).

References:

1. A. Shih, M. Casiulis, S. Martiniani, *Fast generation of spectrally shaped disorder,* Phys. Rev. E, 110(3), 034122 (2024)
2. M. Casiulis, A. Shih, S. Martiniani, *Gyromorphs: a new class of functional disordered materials,* arXiv preprint arXiv:2410.09023 (2024)
3. P. Hoellmer, T. Egg, M.M. Martirossyan, E. Fuemmeler, Z. Shui, A. Gupta, P. Prakash, A. Roitberg, M. Liu, G. Karypis, M. Transtrum, R.G. Hennig, E.B. Tadmor, S. Martiniani, *Open Materials Generation with Stochastic Interpolants*, Proc. 42nd Int. Conf. Mach. Learn. (ICML), PMLR 267 (2025)
4. M. Martirossyan, T. Egg, P. Höllmer, G. Karypis, M. Transtrum, A. Roitberg, M. Liu, R. Hennig, E.B. Tadmor, S. Martiniani, *All that structure matches does not glitter*, accepted at NeurIPS 2025, arXiv:2509.12178 (2025)

TUESDAY, OCTOBER 14, 2025

2:30 PM – 3:30 PM

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