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Invariance to deformations: A new representation for materials space[1] CHANDRAMOULI NYSHADHAM, GUS L. W. HART, Brigham Young University — Huge databases of known materials have been developed using computational and experimental methods over the last century. The existing databases cover a very small fraction of the complete materials space. The future of materials discovery lies in intelligently exploring the materials space (composition and structure space) using machine learning methods. Recently, it has been understood that details of the mathematical representation of materials are key to developing effective algorithms that leverage the machine learning models. One of the main challenges in representing materials space is to incorporate the "deformation stability"— that is small changes in the material imply small changes in representation—a kind of "differentiability". The well-known Fourier based approaches for representing materials space cannot handle the invariance to deformations. In this talk, we will present a new, easy to understand representation based on scattering transforms. Scattering transforms are formally stable to deformations and more effective in interpolating the materials space than the Fourier based approaches. Machine learning models based on scattering transforms offer the potential of high accuracy at the speed of machine learning, thus accelerating materials discovery.

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