

Machine learning for discovery of meaningful chemical and physical contributors to piezoresponse force microscopy

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From high dielectric permittivity and piezoresponse to the pyroelectric and electrocaloric response, ferroelectrics possess a broad range of functionalities. Complex and correlated characterization approaches at multiple length scales have been developed to tackle some of the most challenging questions about the origin of the functional response in ferroic and multiferroic materials. However, data generated through such methods is also of large complexity, and only allows limited insight from direct inspection and traditional statistical analysis. The recent developments in applications of machine learning techniques to materials science offer a path forward, providing powerful new approaches to handle and analyze the information. Specifically, clustering and dimensional reduction techniques are often used as immediate, low computation cost approaches to identify superimposed physical and chemical contributors to functional behavior within multidimensional datasets.

Here, I will provide an overview of machine learning methods applied to characterization of ferroelectric materials through piezoresponse force microscopy (PFM), and particularly the resonant PFM approaches. I will specifically discuss data curation to apply physical and chemical constraints to machine learning, as well as a method to mask or enhance different contributions to the signal.