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From organized high throughput data to phenomenological theory: The example of dielectric breakdown CHIHO KIM, University of Connecticut, GHANSHYAM PILANIA, Los Alamos National Laboratory, RAMPI RAMPRASAD, University of Connecticut — Understanding the behavior (and failure) of dielectric insulators experiencing extreme electric fields is critical to the operation of present and emerging electrical and electronic devices. Despite its importance, the development of a predictive theory of dielectric breakdown has remained a challenge, owing to the complex multiscale nature of this process. Here, we focus on the *intrinsic* dielectric breakdown field of insulators—the theoretical limit of breakdown determined purely by the chemistry of the material, *i.e.*, the elements the material is composed of, the atomic-level structure, and the bonding. Starting from a benchmark dataset (generated from laborious first principles computations) of the intrinsic dielectric breakdown field of a variety of model insulators, simple predictive phenomenological models of dielectric breakdown are distilled using advanced statistical or machine learning schemes, revealing key correlations and analytical relationships between the breakdown field and easily accessible material properties. The models are shown to be general, and can hence guide the screening and systematic identification of high electric field tolerant materials.

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