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Dissolving the Periodic Table in Zirconia: Data Mining for Insight BRYCE MEREDIG, CHRIS WOLVERTON, Northwestern University — A standard approach to understanding physical phenomena in materials is to manually search for clear trends or correlations in data (i.e., descriptors) governing those materials. Pettifor maps are a classic example of such empirically constructed models. But what if a data set is too large and/or chemically diverse to explain by straightforward human inspection? We present such a case by calculating from first principles the solubility thermodynamics of 70 dopant cations in cubic zirconia. This data set, spanning three charge states and most non-synthetic metals in the periodic table, defies simple "manual" explanation. Instead, we employ data mining algorithms and statistical methods to cluster the dopants into distinct classes, and then to build intuitive models for each class' thermodynamics in zirconia. Thus, we show that formal data mining techniques are a powerful means of elucidating meaningful property relationships in complex data sets.

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