Application of artificial neural networks to development of ferroelectric materials

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This study describes a practical application of artificial neural network in combinatorial chemistry. Artificial neural networks are applied to the optimal composition design of ferroelectric materials. This ferroelectric material consists of five components, Bi, Ce, La, Ti, and O. Among five components, the concentrations of Ti and O are fixed. So, the weight percentages of the rest components (Bi, Ce, La) are used as inputs of neural network. The remanent polarization (Pr) and coercive field (Ec) that represent the characteristics of ferroelectric materials serve as the outputs. This neural network is used to model the relationship between the material compositions and the material performances. The proposed model is then used to predict the maximum performance of multi-component material, thereby accelerating the discovery of the optimum composition of ferroelectric material.

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