First Principles Identification of New Cathode Electrocatalysts

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Solid oxide fuel cell (SOFC) performance is limited by poor oxygen reduction kinetics, necessitating identification of new cathode materials. However, their identification is impeded by the combinatorial nature of the problem, the narrow range of good existing SOFC cathode compositions, and by lack of a suitable approach for predicting the efficacy of cathode electrocatalyst candidates. The approach being taken involves development of a correlational model relating a cathode performance metric to various descriptors, e.g., the rate of oxygen exchange is related to surface (and atomistic) descriptors and the model applied using artificial neural networks (ANNs). This approach allows new areas of composition space to be searched using existing data.

The above approach identified physicochemical descriptors and correlated them with performance figures of merit, e.g., surface oxygen exchange rate, using a model encoded into an ANN. The model developed utilized properties of transferability and superposability of unary metal oxides. This enabled prediction of the performance of unary as well as of more complex metal oxides. Consequently, a number of new metal oxide systems were identified for investigation as cathode electrocatalysts. These possess predicted surface oxygen exchange rates comparable to or greater than those of existing and established cathode materials.