

Special Issue

Perovskites in Catalysis and Electrocatalysis

Message from the Guest Editors

Perovskite oxides are a family of functional metal oxides with a general formula of ABO_3 , where the larger A-site cations are commonly rare-earth or alkaline earth metals with 12-fold oxygen coordination, and the smaller B-site cations are commonly transition metals with 6-fold oxygen coordination. More than 90% of the elements in the periodic table can be doped into the A, B, or O sites, leading to a large family of oxides with highly diversified properties. The flexibility of the chemical versatility and crystal structure of perovskites can be used to establish design principles for highly active, selective, and stable (electro)catalysts. Through careful material design of perovskites, the electronic structure can be tuned according to the thermodynamic energies of a variety of reactions to minimize chemical and electrochemical reaction barriers. Bridging perovskite electronic structure with catalysis has promoted comprehensive understanding of catalytic processes, such as surface energetics, activity trends, molecular orbital descriptors, and catalytic mechanistic insights.

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