Proton Conduction in Perovskite Oxides: A Density Functional Theory (DFT) Approach

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Proton-conducting perovskites can be used for fuel cell electrolytes and tritium separation at nuclear plants. Density Functional Theory (DFT) calculations were performed to investigate the mechanisms of proton transport in perovskite oxides. Specifically, the role of native point defects were examined. This talk will provide a practical guidance for design of proton-conducting perovskites using first-principles calculation.