Rational Design of Perovskite-Type Oxides Using First-Principles Modeling

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Computational materials design using density functional theory (DFT) plays an increasingly important role in solving complex problems or challenges in the field of chemical engineering. This presentation will provide an overall idea to rationally design of perovskite-based oxides using first-principles calculation. The two areas will be discussed: 1) Studies on investigation of useful dopants of proton-conducting perovskite, and 2) The role of native point defects in perovskite.