Engineering of cation stability for highly stable and active perovskite-based SOFC electrode materials

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Perovskite-based oxides have been widely used to electrode materials in solid oxide fuel cells (SOFCs). However, rearrangement of cations (e.g., segregation and ex-solution) significantly affects the activity and stability of SOFC under operating conditions. Interestingly, both A-site cation segregation and B-site cation ex-solution phenomena are commonly related to the breaking of cation-oxygen bonds in oxide materials for the cation's segregation toward the surface. Therefore, controlling of cation-oxygen bond strength is an effective way to engineer cation segregation for designing the highly stable and active electrode materials in SOFC.

In this presentation, we first introduce how to understand A-site and B-site cation stability in perovskite materials at the atomic scale using density functional theory (DFT) calculations with the experimental validations. Then, we demonstrate the application of cation stability, such as iso-valent doping, to practically control cation stability in perovskite materials to improve the activity and stability of SOFC electrode materials.