Prediction of Dopant Cation Segregation on $LaBO_3$ Perovskite Oxides from Simple Descriptors

권형욱, 한정우†
서울시립대학교
(jwhan@uos.ac.kr†)

$LaBO_3$ perovskite oxides have attracted great interest for solid oxide fuel cells (SOFCs) cathode materials due to their good oxygen ion-electron conductivity and chemical compatibility with solid-state electrodes. Dopant cation segregation phenomena, however, on the perovskite surfaces deteriorates SOFC cathode performance. It is therefore important to suppress the dopant segregation. Unfortunately, the origin of the dopant segregation on perovskite oxides has not been yet clear. In this study, we performed density functional theory (DFT) calculations to investigate key thermodynamic driving forces of the segregation at the atomic level. Our results showed that the elastic energy minimization of dopant cations plays an important role to dopant segregation. Furthermore, we suggested useful descriptors for predicting the segregation behavior through intrinsic information of the materials. We believe that our results will be essential to design new cathode materials that can effectively suppress the dopant segregation.