Theoretical Study of the Effect of Anion Doping in Perovskite Oxide for Varying Dielectric Constant

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Multilayer ceramic capacitor (MLCC) is the representative passive element that plays a key role in electronic circuits and the market demand on MLCC is ever increasing. Especially, the performance of MLCC can be improved by doping of heterogeneous elements on the dielectric material. Current studies have focused on tuning physical properties by the substitution of cation even though there are insufficient numbers for candidates that can be synthesized by cationic substitution. Thus, we propose anion substitution to be a new alternative strategy. In this study, the effects of anion doping on perovskite oxides were investigated by density functional theory calculations. ABO3 type perovskite oxides were modeled with difference types of dopants for the substitution of their O-sites were considered. The feasibility of each dopant substitution was investigated via doping formation energy and dielectric constant. In addition, ideal candidates with high dielectric constant were drawn by the difference in comparison of their density of states.