

Abstract Submitted
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***p*-doped BiFeO₃ - a survey of the periodic table** JULIAN GEBHARDT, ANDREW RAPPE, University of Pennsylvania, Department of Chemistry, RAPPE GROUP TEAM — We provide a comprehensive study of substitutional metal doping in multiferroic BiFeO₃ (BFO) by *ab initio* calculations. The study focuses on *p*-type doping, since, to date, no successful *p*-doped modification has been reported, impeding its use in electronic applications. Despite the resulting focus on M^{+*n*<3} cations, we also discuss isovalent and aliovalent *n* dopants. The resulting set of candidates spans the most part of the periodic table and we investigate the possibility and the effects on the electronic structure of substitutional doping in both A- (Bi) and B-site (Fe) for each dopant. We are able to establish trends and to identify suitable *p* dopants in both possible doping sites. Furthermore, we extend our study in order to incorporate the effects of oxygen vacancies on the electronic structure. This is the most important structural defect in BFO as oxygen vacancies, which are present in most experimentally grown crystals, inherently lead to *n* doping of the material. We find that the formation of oxygen vacancies depends on the oxidation state of the dopant but also deviations within groups of the same oxidation state are observed. This allows us to rank all *p* dopants with respect to their tendency to limit oxygen vacancy formation.

Julian Gebhardt
University of Pennsylvania, Department of Chemistry

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