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Accelerated materials design of fast oxygen ionic conductors based on first principles calculations XINGFENG HE, YIFEI MO, Department of Materials Science and Engineering, University of Maryland, College Park — Over the past decades, significant research efforts have been dedicated to seeking fast oxygen ion conductor materials, which have important technological applications in electrochemical devices such as solid oxide fuel cells, oxygen separation membranes, and sensors. Recently, $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) was reported as a new family of fast oxygen ionic conductor. We will present our first principles computation study aims to understand the O diffusion mechanisms in the NBT material and to design this material with enhanced oxygen ionic conductivity. Using the NBT materials as an example, we demonstrate the computation capability to evaluate the phase stability, chemical stability, and ionic diffusion of the ionic conductor materials. We reveal the effects of local atomistic configurations and dopants on oxygen diffusion and identify the intrinsic limiting factors in increasing the ionic conductivity of the NBT materials. Novel doping strategies were predicted and demonstrated by the first principles calculations. In particular, the K doped NBT compound achieved good phase stability and an order of magnitude increase in oxygen ionic conductivity of up to 0.1 S cm^{-1} at 900 K compared to the experimental Mg doped compositions. Our results provide new avenues for the future design of the NBT materials and demonstrate the accelerated design of new ionic conductor materials based on first principles techniques. This computation methodology and workflow can be applied to the materials design of any (e.g. Li+, Na+) fast ion-conducting materials.

Xingfeng He
Univ of Maryland-College Park

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