

Unusual aspects of ion migration in perovskites

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Abstract

The transport of ions in ABO_3 perovskite materials has been studied for decades, and ion transport within the lattice is considered to be relatively well characterised and understood. This is not the case, however, for ion transport along dislocations in perovskites. Even for the most well-studied system, $SrTiO_3$, the story of oxygen diffusion is long and tortuous, and it is only recently that a consistent picture has emerged. In the case of cation diffusion along dislocations in perovskites, the story is short and incomplete (the only published study dates back to the 1960's). In my talk, I will discuss recent work on measuring and simulating ion diffusion along dislocations in the perovskites $SrTiO_3$ and $BaTiO_3$. I will emphasise that lattice diffusion has to be understood before dislocation diffusion can be studied, and that the presence of space-charge zones at extended defects needs to be considered. In addition, I will demonstrate the strengths of combining a variety of experimental and computational techniques.

Biography

Roger A. De Souza obtained a B. Eng in Material Science and Engineering in 1992 and a Ph.D. in Materials Science in 1996 from Imperial College London. After spending two years as a post-doctoral researcher at the University of Karlsruhe, he moved to the Max-Planck Institute for Solid State Research in Stuttgart. In 2002 he joined the Institute of Physical Chemistry at RWTH Aachen University, where he received his professorial degree (Habilitation) in 2011 and was promoted to Professor in 2017. The De Souza group performs fundamental research, encompassing both experimental and computational approaches, on complex oxides for energy and information technologies. One particular theme is characterising and understanding transport processes in these oxides and at their extended defects.