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Anion and cation diffusion in complex oxides

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Oxygen diffusion in complex oxide materials is of great importance for applications, e.g. in fuel cells (oxygen ion conductivity) or oxygen permeation membranes (ambipolar diffusion of oxygen). For heavily doped oxides, such as doped zirconia, ceria or lanthanum gallate, we give a qualitative and quantitative explanation of the observed maximum of the conductivity as a function of the dopant fraction by combining DFT calculations of energies and entropies with kinetic Monte simulations of the oxygen ion conductivity. Concerning cation diffusion in complex oxides, we report our recent findings in perovskites, with a special focus on doped lanthanum gallate, barium titanate, and BSCF. Our experimental results indicate that the cation diffusion mechanisms are more complicated than simple vacancy mechanisms. We show that the experimental observations can be explained well by A- and B-site cation vacancies that are strongly bound in defect clusters and perform a highly correlated motion.

Biography

Manfred Martin is a Professor and Head of the Institute of Physical Chemistry of RWTH Aachen University, Germany. He has more than 30 years of experience in education and research of physical chemistry of solids. His current research focusses on materials for energy conversion, resistive switching, solid-state reactions, secondary ion mass spectrometry, and computer simulations as well. He has published >200 scientific papers in international, refereed journals. He received Carl-Wagner Award and has been elected as member of the Royal Society of Chemistry. He has supervised more than 50 PhD students and more than 20 postdoctoral fellows.

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