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Diffusion in Oxides – from Fuel Cells to Memristors

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Interest in materials exhibiting oxygen ion conduction and/or mixed ionic-electronic conduction has increased during the last years owing to their great importance for energy and environmental applications, such as solid oxide fuel cells for converting chemical to electrical energy, solid oxide electrolyser cells for high-temperature electrolysis of water, and oxygen permeation membranes for separating oxygen from air. While the above diffusion processes take place on a macroscopic or mesoscopic scale oxygen diffusion on the nanoscale is important for memristic devices. In these metal-insulator-metal structures diffusion of oxygen due to an external electric bias modulates the resistance of the devices and renders possible multilevel resistive switching being the basis for neuromorphic computing.

Ceria-based oxides are regarded as key oxide materials for the above energy applications due to the fact that rare earth-doped ceria is a pure oxygen ion conductor while undoped ceria is a mixed oxygen ion–electron conductor. We will discuss our *ab initio* studies of oxygen diffusion in these materials based on density-functional theory (DFT) and Kinetic Monte Carlo (KMC) simulations [1,2]. In thin films of amorphous gallium oxide sandwiched by two ion-blocking electrodes we found memristic behaviour caused by homogeneous migration of ions and their electrochemical polarization [3,4]. We will discuss the underlying mechanisms and compare with the often found filamentary switching mechanism.

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[4] C. Kura, Y. Aoki, E. Tsuji, H. Habazaki and M. Martin, RSC Advances, 6, 8964 (2016).