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ABSTRACT

Mass and Charge Transport in Oxides – from Energy Conversion to Memristic Devices

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Interest in materials exhibiting ionic conduction 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 chemical reactions. In memristic devices transport of ions due to an external electric bias modulates the electronic conductivity of the devices and renders possible multilevel resistive switching being the basis for neuromorphic computing.
Perovskite oxides are regarded as key materials for the above energy applications and for memristic devices as well. We will discuss our *ab initio* studies of proton and oxygen ion transport in doped $BaZrO_3$ based on density-functional theory (DFT) and Kinetic Monte Carlo (KMC) simulations [1,2]. In $SrTiO_3$ we found memristic behaviour triggered by transport of oxygen ions and resulting in filamentary switching or bulk switching depending on the experimental conditions [3,4]. Finally, we will discuss or recent findings on variable-range hopping of electrons in amorphous gallium oxide that shows bulk resistive switching [5].

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