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Structural changes induced by stoichiometry deviation and related properties in binary oxides

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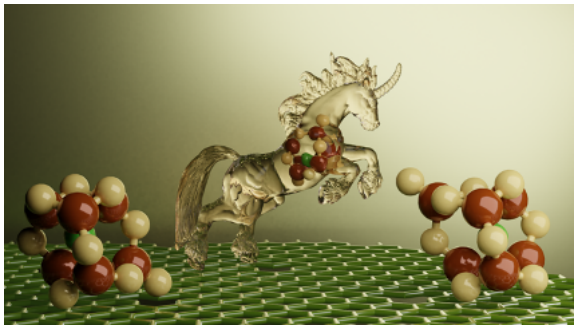

Binary transition metal oxides are considered to be prospective for the next generation highly scalable memory devices and neuromorphic computing due to the memristor-like behavior and resistive switching phenomena. The physical origin of the mechanism behind the resistive switching includes oxygen vacancy migration, trapping of charge carriers, spatial inhomogeneity, Schottky barriers, interfaces, filamentary paths formation. Among binary oxides the HfO_2 is of special interest due to its excellent CMOS compatibility: hafnium-based dielectrics were already utilised as high-k oxides for metal-oxide-semiconductor field-effect transistors (MOSFET). In addition to resistive switching ability, recently discovered ferroelectricity in Si:HfO_2 thin films [1], which can be scaled down to sub-2 nm thickness [2], extends the functionality of the hafnia-based memory devices. Reported ferroelectricity in undoped HfO_2 [3] emphasizes the importance of oxygen deficiency not only for resistive switching, but also for the desired ferroelectric properties and requires its better microscopical understanding. It is noteworthy that HfO_2-based (anti-)ferroelectrics are also high-capacity energy storage materials [4], which in principle enables design of system-on-a-chip devices with data storage, signal processing, in-memory computing, neuromorphic computing, amplifiers and power suppliers using only one CMOS-compatible active oxide. To understand different behavior of oxygen vacancies in various oxides, we investigated phase diagrams of Hf-O, Zr-O, Y-O, Ta-O and Nb-O solid solutions using evolutionary algorithm [5] in combination with ab initio methods. We discuss the difference in structural changes induced by deviation of stoichiometry from that of the pristine thermodynamically stable compounds and illustrate the role of oxygen vacancy ordering on the resistive switching [6,7] and on ferroelectricity in HfO_2 [8]. We will present the results of structural simulation of small Hf_nO_x (n=3-10) clusters and discuss the local changes in the structures, induced by off-stoichiometry in pure HfO_x clusters and their mediation by C dopants [9].

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[1] T. Böscke et al., Appl. Phys. Lett. **99**, 102903 (2011); [2] H. Lee et al, ACS Appl. Mater. Interfaces **13**, 36499-36506 (2021); [3] P. Polakowski, J. Müller, Appl. Phys. Lett. **106**, 232905 (2015); [4] F. Ali et al., J. Appl. Phys. **122**, 144105 (2017); [5] http://uspex-team.org; [6] K.Z. Rushchanskii, S. Blügel, M. Ležaić, Phys. Rev. Materials **2**, 115002 (2018); [7] K.Z. Rushchanskii, S. Blügel, M. Ležaić, Faraday Discuss. **213**, 321-337 (2019); [8] K.Z. Rushchanskii, S. Blügel, M. Ležaić, Phys. Rev. Lett. **127**, 087602 (2021); [9] N. Schmidt, K.Z. Rushchanskii, U. Trstenjak, R. Dittmann, S. Karthäuser, submitted to Nanoscale (2022).