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Ab initio Calculations for Hydrogen-Doped HfO_{2-x} RRAM DAN DUNCAN, BLANKA MAGYARI-KOPE, YOSHIO NISHI, Stanford University — Hydrogen impurities are shown to have significant effects on the mechanism of electronic conduction in HfO_2 -based resistance change memory (RRAM) devices, and to affect the ionic transport during the forming, set, and reset processes. Using density functional theory and employing the LDA+ U formalism, the diffusion of oxygen ions in hydrogen-doped HfO_{2-x} was examined and its implications on the electronic structure are determined. Results indicate that hydrogen can have multiple substantial effects on device operation, and has a strong potential to improve device switching and uniformity. These hydrogen-doped devices make promising candidates for low-voltage and forming-free memory schemes, as well as for electronic synapses in neuromorphic systems.

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