Ab-initio-parametrized kinetic Monte Carlo model for vacancy diffusion in amorphous oxides in valence change memory cells

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One of the most promising technologies for emerging neuromorphic computing architectures are valence change memory (VCM) cells. Their operational principle relies on the creation (SET process) and the disruption (RESET process) of the conductive filament made of oxygen vacancies. To shed light on these processes, we have developed a fully-atomistic kinetic Monte Carlo (KMC) model. The activation energies of relevant events, namely oxygen vacancy diffusion, oxygen ion diffusion and oxygen vacancy ion-pair generation and recombination, are precomputed using density functional theory calculations. The model then executes the events according to their probabilities, which defines the shape of the filament at the given applied voltage and at the given temperature. The obtained structures are subsequently passed to a quantum transport solver to compute the conductance and the current. We further demonstrate that our model is able to capture relevant processes in a VCM cell, such as filament formation and SET and RESET processes, by applying it to hafnium dioxide-based VCM cells.

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DFTBephy: a DFTB-based approach for electron-phonon coupling calculations

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The calculation of electron-phonon couplings from first principles is computationally very challenging and remains mostly out of reach for systems with a large number of atoms. Resorting to semi-empirical methods, like density-functional based tight-binding (DFTB), has been shown to be a viable approach for obtaining quantitative results at moderate computational costs. Herein, we present a method for calculating the electron-phonon coupling matrix within the DFTB approach and demonstrate its implementation based on DFTB+ and phonopy. Exemplarily, we show results for gamma-graphyne which was recently synthesized [1] consistent with earlier predictions we obtain relaxation times 10-14 s at room temperature.

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Electromagnetic control of electron interference

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Recent advances in electron quantum optics and single electron sources allow the generation of coherent single electrons and enable to engineer coherent manipulations of electrons. Making use of the wave nature of electrons, offers fascinating opportunities in many fields of application, such as quantum information processing, quantum sensing and quantum metrology. Single electron control can be established by specifically shaped potentials, which cause focusing, splitting and interference effects. Here, we apply the Wigner signed-particle method to analyze the focusing properties of the double-well potential structure. The physical setup resembles the Young double-slit experiment, but offers the advantage to control the electrostatic potential of the dopants and thus the interference pattern. Additionally, we apply a uniform magnetic field and analyze its impact. We investigate the electron density and the negativity of the Wigner function to show how the magnetic field controls the electron state but also destroys the coherence of the evolution dynamics.