Abstract Submitted
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Coupled molecular-dynamics and first-principle transport calculations of metal/oxide/metal heterostructures[1] PETER ZAPOL, Argonne Natl Lab, DMITRY KARPEYEV, University of Chicago, KETAN MAHESHWARI, XIAOLIANG ZHONG, BADRI NARAYANAN, SUBRAMANIAN SANKARANARAYANAN, MICHAEL WILDE, OLLE HEINONEN, Argonne Natl Lab, IVAN RUNGGER, Trinity College — The electronic conduction in Hf-oxide heterostructures for use in, e.g., resistive switching devices, depends sensitively on local oxygen stoichiometry and interactions at interfaces with metal electrodes. In order to model the electronic structure of different disordered configurations near interfaces, we have combined molecular dynamics (MD) simulations with first-principle based non-equilibrium Green's functions (NEGF) methods, including self-interaction corrections. We have developed an approach to generating automated workflows that combine MD and NEGF computations over many parameter values using the Swift parallel scripting language. A sequence of software tools transforms the result of one calculation into the input of the next allowing for a high-throughput concurrent parameter sweep. MD simulations generate systems with quenched disorder, which are then directly fed to NEGF and on to postprocessing. Different computations can be run on different computer platforms matching the computational load to the hardware resources. We will demonstrate results for metal-HfO2-metal heterostructures obtained using this workflow.

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