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First-Principles Investigation on Atomic and Electronic Transport in Ag-Ag_2S-Ag ZHONGCHANG WANG, TAKUYA KADOHIRA, TOMOFUMI TADA, SATOSHI WATANABE, Department of Materials Engineering, The University of Tokyo and CREST-JST — A novel atomic switch using Ag-Ag_2S-Ag heterostructure has seized a wide range of attentions recently. Its switching mechanism, however, has not been understood sufficiently. As a first step to clarify the mechanism, we investigated migration pathways of Ag ions and activation energies for the migration in Ag_2S, and then examined the interface structures, electronic states and electric properties of the Ag-Ag_2S-Ag system, using the density functional theory. The calculated activation energies for the migration are between 0.31 to 0.50 eV, which are comparable to the experimental values of 0.43 to 0.48 eV. The calculated transmission coefficient of Ag-Ag_2S-Ag at the Fermi level increases from 0.04 before atomic relaxation to $0.455G_0$ after relaxation, which shows the opening of a conduction channel in the relaxed structure. Further analysis of atomic configuration in the relaxed structure shows formation of a chain-like arrangement of Ag in Ag_2S.

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