Atomic Structures, Electronic States, and Quantum Transport

Properties of Solid Electrolyte Atomic Switches from First-Principles

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Atomic switches using solid electrolyte such as Ag\textsubscript{2}S and Cu\textsubscript{2}S have attracted much attention recently as a promising candidate for nanoscale devices, because of its simple structure, stability and reliability at room temperature, and being easy to transfer to real electronic circuits. Though a lot of intriguing results have already been obtained concerning these switches,\textsuperscript{1-3} their working mechanism have not been well clarified yet. Here, to understand the switch mechanism, we have examined atomic structures, electronic states, and transport properties of Ag\textsubscript{2}S–Ag\textsubscript{2}S–Ag and Cu\textsubscript{2}S–Cu\textsubscript{2}S–Cu systems from first-principles.

The system investigated consists of Ag\textsubscript{2}S (Cu\textsubscript{2}S) layers connected to two semi-infinite Ag (Cu) electrodes. We adopted two types of models for the Ag\textsubscript{2}S system: One has the orientation relationship consistent with experiments but has large lattice mismatch, while the other has a small mismatch but different orientation relationship. For the Cu\textsubscript{2}S system, our model satisfies the observed orientation relationship and has small lattice mismatch. The electronic structures of these models were calculated using Atomistix Toolkit code, which is based on non-equilibrium Green’s function method within the density functional theory.

In the case of the large mismatch model of Ag\textsubscript{2}S–Ag\textsubscript{2}S–Ag system, we found that the transmission coefficient at \( E_F \) increases from 0.04 before structural relaxation to 0.455 after relaxation, which shows the opening of a conduction channel in the relaxed structure.\textsuperscript{4} Further investigation revealed that a zigzag Ag atomic chain is formed in the Ag\textsubscript{2}S, as shown in Fig. 1(a). The electron density of the Ag atomic chain is illustrated in Fig. 1(b). The calculated current-voltage curve is nearly linear, showing metallic nature of this system. On the other hand, such a metallization of Ag\textsubscript{2}S does not occur in the small mismatch model. However, we found that even in this small mismatch model, the system becomes metallic through introducing a certain amount of Ag atoms into the Ag\textsubscript{2}S layer with appropriate arrangements. The occurrence of the metallic nature can be explained by the gradual generation of a conductive Ag bridge inside the Ag\textsubscript{2}S till complete connection to the two Ag electrodes, as shown in Fig. 2.

In the case of the small mismatch model of Cu\textsubscript{2}S system, the above spontaneous metallization after structural optimization has not been observed. However, we found that the addition of certain amount of Cu into the Cu\textsubscript{2}S layers with appropriate arrangement makes these systems...
metallic, in a way that is similar to the small mismatch model of the Ag$_2$S system.

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References


FIG. 1. (a) Atomic arrangement of the relaxed structure of the Bridge case. The numbers denote the neighboring Ag–Ag distances along the chain in the Ag$_2$S. (b) Electron density corresponding to the atoms along the chain.

FIG. 2. Evolution of a bridge formation inside the Ag$_2$S with the introduction of excess Ag atoms.