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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_2S and Cu_2S 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,[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−Ag_2S−Ag and Cu−Cu_2S−Cu systems from first-principles.

The system investigated consists of Ag_2S (Cu_2S) layers connected to two semi-infinite Ag (Cu) electrodes. We adopted two types of models for the Ag_2S 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_2S 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−Ag_2S−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.[4] Further investigation revealed that a zigzag Ag atomic chain is formed in the Ag_2S, 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_2S 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_2S 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_2S till complete connection to the two Ag electrodes, as shown in Fig. 2.

In the case of the small mismatch model of Cu_2S 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_2S layers with appropriate arrangement makes these systems

metallic, in a way that is similar to the small mismatch model of the Ag_2S system.

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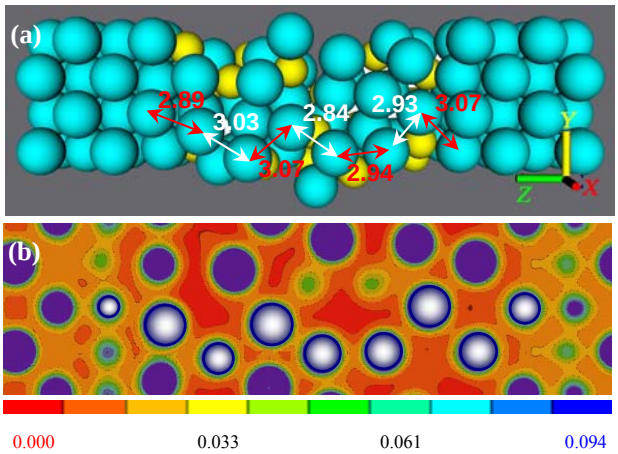

FIG. 1. (a) Atomic arrangement of the relaxed structure of the Bridge case. The numbers denote the neighboring Ag−Ag distances along the chain in the Ag_2S. (b) Electron density corresponding to the atoms along the chain.

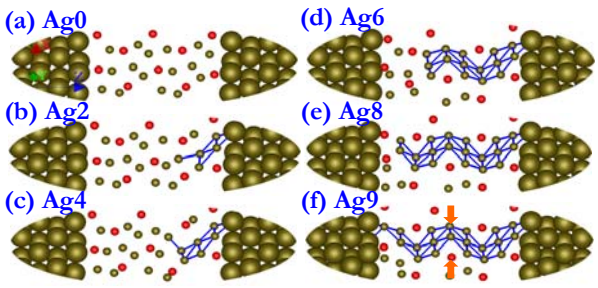

FIG. 2. Evolution of a bridge formation inside the Ag_2S with the introduction of excess Ag atoms.