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Ab initio non-equilibrium Green's function study on the growth of metallic bridge in mixed conductor atomic switch TOMOFUMI TADA, ZHONGCHANG WANG, TINGKUN GU, SATOSHI WATANABE, Dept. of Materials Engineering, The Univ. of Tokyo, JST-CREST — A novel atomic switch [1] composed of a mixed conductor, Ag_2S or Cu_2S, has attracted much attention. To investigate the electronic properties of the atomic switch, we have examined interface structure and electron transport of $Ag/Ag_2S/Ag$ and $Cu/Cu_2S/Cu$ using ab initio non-equilibrium Green's function method. In $Ag/Ag_2S/Ag$, we found a spontaneous growth of a metallic bridge composed of a Ag atomic chain when a unidirectional stress is applied to Ag_2S [2]. On the contrary, a metallic bride does not appear in Ag_2S and Cu_2S without stress. We also examined the influence of Ag/Cu addition on the structural and transport properties of Ag_2S and Cu_2S atomic switches, and found that the Ag/Cu addition leads to the metallization in the both systems. However, clear growth of the atomic bridge is confirmed only in $Ag/Ag_{2+\delta}S/Ag$. The metallic nature in $Cu/Cu_{2+\delta}S/Cu$ is related to the growth of electron charge network at the Fermi level. 1) K. Terabe, et al., Nature 433, 47 (2005). 2) Z. Wang, T. Kadohira, T. Tada, S. Watanabe, Nano Letters 7, 2688 (2007).

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