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First-principles study of electronic transport properties of Ta_2O_5 atomic switch[1] SATOSHI WATANABE, TINGKUN GU, TOMOFUMI TADA, Department of Materials Engineering, The University of Tokyo, COMPUTATIONAL MATERIALS SCIENCE LAB TEAM — The atomic switch using solid electrolyte such as Ta_2O_5 has attracted attention as a promising novel nanoscale device. In the case of the Ta_2O_5 switch, experiments shows that the precipitation of metal in the Ta_2O_5 layer plays a crucial role in forming the low resistance state of the switch. However, atomistic details of the conduction path have not been clarified yet. In this work, we have examined the electronic transport properties of the low resistance state of the $Cu/Ta_2O_5/Pt$ atomic switch using the density functional theory (VASP code) and non-equilibrium Green's function method (ATK code). Our results show that a Cu chain bridging Cu and Pt electrodes works as a conduction path in the case of crystalline Ta_2O_5. On the other hand, preliminary results show that the conduction through similar Cu chain structures is unexpectedly low in the case of amorphous Ta_2O_5.

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