Al Conducts Better than Cu at the Atomic Scale: A First-Principles Study of Metallic Atomic Wires

Adam J. Simbeck[1,‡,*], *Nick Lanzillo*[1,‡], *Neerav Kharche*[1,2], *Matthieu J. Verstraete*[3], *and Saroj K. Nayak*[1]

[1]Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY, 12180, USA

[2]Computational Center for Nanotechnology Innovations, Rensselaer Polytechnic Institute, Troy, NY 12180, USA

[3]Nanomat unit, Department of Physics, University of Liege, B-4000 Liege, Belgium

Corresponding Author

*simbea@rpi.edu

Supporting Information

The application of an external electric field has a negligible effect on the electronic states of the atomic wire (Figure S.1). For example, for an N = 5 Cu atomic wire a field of 0.0019 au (1.0 V bias) shifts the majority of the energy levels by less than 0.1 eV. Any levels that see a dramatic change are far in energy from the highest occupied molecular orbital (HOMO) such that they are not involved in the transport calculation. Similar modifications of the electronic energy levels of the atomic wire are seen for the other metals considered, *i.e.,* Al, Ag, and Au.

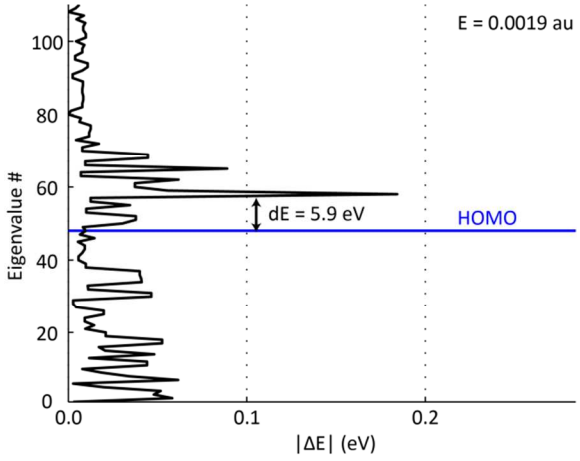

Figure S.1 Effect of an applied external field on the electronic states of an N = 5 Cu atomic wire. Significant shifts in the energy levels due to the applied field only occur for states far from those involved in transport.

By increasing the size of the contacts, we can in principle get a more accurate description of the self-energy matrices of the contacts but this does not affect the trends in our quantum transport calculations. As shown in the figure below (Figure S.2), the inclusion of more atoms in the contacts preserves the trend of Al performing better than Cu and only shifts the IV plots by at most ~6 μA. The trend is also preserved for contacts of larger width. The example shown is for a

N = 5 Cu wire with Au contacts which have been extended in the [111] direction to include 20 atoms.

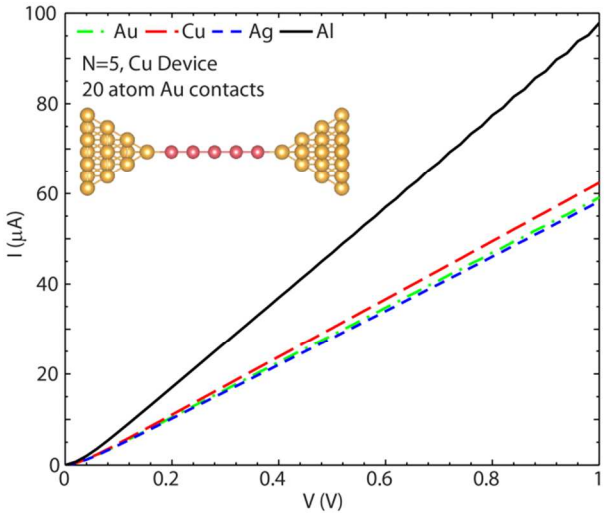

Figure S.1 Effect of contact on quantum transport current *vs.* voltage. The use of larger contacts (20 Au atoms) does not significantly alter the results of the transport calculation. Rather the general trends are preserved. The example shown is for an N = 5 Cu atomic wire with 20 atom pyramidal Au contacts built in the [111] direction.