Theoretical Study of Conductance through Monoatomic Nanowires

Mirzaeva Irina V.,[1,2] Kozlova Svetlana G.[1,2]

[1] *Nikolaev Institute of Inorganic Chemistry SB RAS, Lavrentieva 3, 630090, Novosibirsk, Russia*

[2] *Department of Natural Sciences, Novosibirsk State University, Pirogova 1, 630090, Novosibirsk, Russia*

* *E-mail: dairdre@gmail.com*

Molecular electronics attract an increasing interest of researchers from various fields of science. Advances in the field of cluster chemistry make it possible to synthesize systems that can be considered as promising molecular devices [1]. However, modeling of electronic transport through such systems is a rather difficult task. A common simplification is the use of monoatomic wires as electrodes. However, the properties of the monoatomic nanowires themselves are not yet sufficiently studied.

Here we present theoretical studies of geometry, electronic structure and transport properties of Cu, Ag, Au and Pt monoatomic nanowires. Geometry and electronic structure were studied using BAND 2021 program [2] including both, scalar and spin-orbit levels of relativistic corrections. Transport properties of monoatomic nanowires between bulk electrodes (Fig. 1) were studied with SIESTA package [3] using non equilibrium Greens functions approach including only scalar relativistic effects.

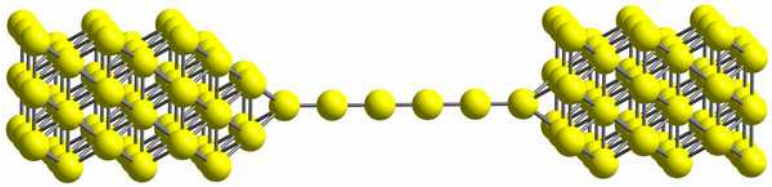

Figure 1. Monoatomic nanowire between bulk contacts.

The work was supported by the Russian Science Foundation, project №22-23-00245.

[1] S.P. Gabuda, S.G. Kozlova, Yu.V. Mironov, V.E. Fedorov, *Nanoscale Res Lett* **2009**, *9*, pp. 1110–1114.

[2] BAND 2021, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com

[3] SIESTA 4.1.5, http://siesta-project.org/