RSC Advances

This article can be cited before page numbers have been issued, to do this please use: R. Šedivá, K. Mašek, M. E. Pronsato and C. Pistonesi, *RSC Adv.*, 2016, DOI: 10.1039/C6RA16993G.

ROYAL SOCIETY OF CHEMISTRY

www.rsc.org/advances

View Article Online
DOI: 10.1039/C6RA16993G

Tungsten oxide nanowire on copper surfaces: a DFT model

R. Šedivá[1], K. Mašek[1], M.E. Pronsato[2], C. Pistonesi[2*]

[1] Charles University in Prague, Dept. of Surface and Plasma Science, V Holešovičkách 2, 180 00 Prague 8, Czech Republic

[2] IFISUR, Universidad Nacional del Sur, CONICET, Departamento de Física UNS, Av. L. N. Alem 1253, Bahia Blanca, Argentina.

*Corresponding author: carolina.pistonesi@uns.edu.ar

Tel- fax: +54 0291 4595142

View Article Online
DOI: 10.1039/C6RA16993G

ABSTRACT

We studied a model of a one dimensional tungsten oxide nanowire on reconstructed Cu(110) surface by Density Functional Theory calculations. The effect of oxygen vacancies on the electronic structure was analyzed (DOS). Nanowire equilibrium geometric configuration corresponds to tungsten oxide strips oriented along Cu [1-10] direction, in which W-W distances are similar to the bulk data, in agreement with electron diffraction experiments. Bader charge analysis shows that electron charge of W atoms corresponds to a tungsten atom in 6+ oxidation state. The presence of the oxygen vacancies increase the electronic charge of tungsten atoms. Formation of the oxygen vacancies by removal of terminal oxygen atoms is energetically favorable. Calculated PDOS shows stabilization of tungsten states to lower energies due to the presence of oxygen vacancies.

KEYWORDS: tungsten oxide, nanowires, oxygen vacancies, DFT