Accepted Manuscript

Influence of CO molecule on structure stability and electronic properties of silver nanotube

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PII: \$0577-9073(17)30492-6

DOI: https://doi.org/10.1016/j.cjph.2018.07.008

Reference: CJPH 589

To appear in: Chinese Journal of Physics

Received date: 25 April 2017 Revised date: 4 May 2018 Accepted date: 20 July 2018



Please cite this article as: Liang-Cai Ma, Xi-Zhi Wang, Jian-Min Zhang, Influence of CO molecule on structure stability and electronic properties of silver nanotube, *Chinese Journal of Physics* (2018), doi: https://doi.org/10.1016/j.cjph.2018.07.008

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Highlights

- The top and bridge (B1) sites are the stable sites for CO molecule adsorption.
- The AgNT undergoes a slight structural distortion after the CO adsorption.
- The electronic structure properties can be described by the Blyholder model.
- The quantum conductance of AgNT decreases by $1G_0$ after CO adsorption.



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