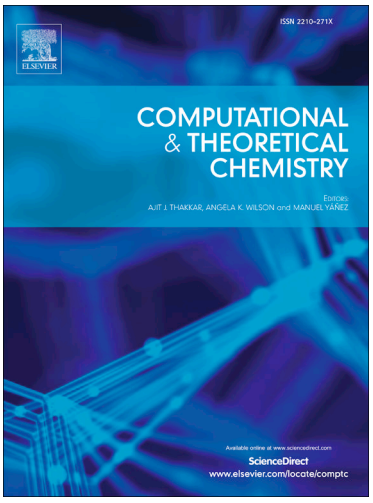

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First-principles investigation on vibrational properties of coinage metal (4, 2) nanotubes

Aping Yang[*,‡], Dongming Li[*], Yankun Zhen[*], Guoxiang Chen[*], Ping Guo[†]

** School of Science, Xi'an Shiyou University, Xi'an 710065, P. R. China.*

† *Department of Physics, Northwest University, Xi'an 710069, P. R. China.*

‡ *yangap@xsyu.edu.cn*

Using first-principles calculations, we have investigated the structural stabilities, electronic and vibrational properties of the (4, 2) single-walled coinage metal nanotubes, especially the Raman-active radial breathing modes (RBMs). It is found that 1) the tip-suspended (4, 2) single-walled coinage metal nanotubes may also be grown in future, because of the appearance of local minimums in the string tensions and binding energies variation with the lengths of unit cell. 2) The different coinage metal (4, 2) nanotubes have different characteristic RBMs, whose frequencies correspond exactly to their maximal frequencies. In addition, the vibrational density of states depends on both of their elements and the structural symmetries. 3) The calculated stiffness coefficients of the coinage metal (4, 2) tubes further indicate that their bond strengths are different from each other, for which the Cu-Cu bond is harder than both of the Au-Au and Ag-Ag bonds. 4) The available resonant Raman spectra of their RBMs are sensitive to the species of nanotubes, which may be useful for identifying them in possible experiments.

Keywords: Coinage metal (4, 2) nanotubes, First principles, First-order resonant Raman spectra, Radial breathing modes

[‡]Corresponding author:yangap@xsyu.edu.cn