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First Principle Study on Wurzite Core-shell Nanowires Heterostructures ZnO/ZnS. TUOC VU[1], University of Illinois Urbana-Champaign, Dep. of Materials Science & Engineering, 1304 W. Green, Urbana, IL, USA — We present a first-principle study on the structural and electronic structure of II-VI wurtzite core-shell core-multishell ZnO/ZnS hexagonal unsaturated and saturated nanowire and examine the dependence of interface stress and formation energy on nanowire lateral size with diameter range from 20Å up to 36.4Å. We also calculated Young's modulus along growth direction and tensile test have been applied for various wires to show the diameter dependence's of their mechanical properties. The electronics properties of heterostructure nanowire (e.g. band structure, Density of State, charge transfer via Mulliken population analysis) also exhibit wire's diameter dependence behaviors..

[1]On leave from Hanoi University of Technology, Institute of Engineering Physics Hanoi 10000, Vietnam

Tuoc Vu
University of Illinois Urbana-Champaign, Dep. of Materials Science
& Engineering, 1304 W. Green, Urbana, IL, USA

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