

Abstract Submitted
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Ab-initio study of field emission characteristics of single-walled ZnO nanotubes WEI-CHIH CHEN, FENG-CHUANG CHUANG, ZHI-QUAN HUANG, Natl. Sun Yat-Sen Univ., Taiwan, WAN-SHENG SU, Natl. Center for High-Performance Computing, Taiwan — We employed first-principles calculations to investigate the field emission characteristics of infinite-length single-walled ZnO nanotubes (SWZONTs) in the either armchair or zigzag conformations. Both armchair and zigzag SWZONTs are found to be direct-bandgap semiconductors. Moreover, our calculations demonstrated that work functions of armchair and zigzag tubes decrease from about 5.70 to 5.25 eV with an increasing tube diameter, and it eventually approaches to the work function value of a ZnO sheet with a diameter close to an infinite limit. Finally, the direct computations on field emission factors of both nanotubes will be presented. Our findings provide an insight into the ZONT field-emission properties as well as contribute to developing procedures to produce an efficient ZONT field emitter.

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