

Abstract Submitted
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Electronic structures of MoS₂ nanotubes. LINGYUN XU, MURRAY DAW, XING GAO, ERDI BLEDA, Clemson University — The electronic structure of MoS₂ nanotubes has been studied using first principles. We investigated MoS₂ zigzag (n, 0) nanotubes as well as armchair (n, n) structure. We constructed MoS₂ nanotube with ABA and ABC stacking. The structures have been completely optimized. We compare to previous tight-binding calculations by Seifert et al.(Phys. Rev. Lett. 85, 146 (2000)).

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