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First-principles investigation of electronic band gap in multi-walled carbon nanotube: Role of mechanical deformations PAVAN K. VALAVALA, Department of Physics and Mechanical Engineering-Engineering Mechanics, Michigan Technological University, GREGORY M. ODEGARD, Department of Mechanical Engineering-Engineering Mechanics, Michigan Technological University, RANJIT PATI, Department of Physics, Michigan Technological University, Houghton, MI 49931 — The carbon nanotube (CNT) structures have been the subject of intense research in recent years. Some studies have shown that the electronic band gap in single walled CNT can be modulated through mechanical deformations such as flattening. It has been shown that single walled CNTs undergo a semiconducting-metallic and semiconducting-metallic-semiconducting transition when subjected to deformations. However, the modulation of electronic band gap of multiwalled CNT under mechanical deformations has not been studied. We have used first- principles gradient density functional approach to explore the role of flattening on the electronic properties of MWCNT structures. The influence and the effect of flattening on the electronic properties of the constituent single walled CNTs are also explored.

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