Abstract Submitted for the MAR07 Meeting of The American Physical Society

Dielectric Response and Born Dynamic Charge of BN Nanotubes from Ab Initio Finite Electric Field Calculations GUANG-YU GUO, Department of Physics, National Taiwan University, Taipei 106, Taiwan, SHOJI ISHIBASHI, TOMOYUKI TAMURA, Research Institute for Computational Sciences, National Institute of Industrial Science and Technology, Tsukuba, Japan, KIYOYUKI TERAKURA, Creative Research Institute "Sousei", Hokkaido University, Sapporo, Japan — Since the discovery of carbon nanotubes (CNTs) in 1991 by Iijima, carbon and other nanotubes have attracted considerable interest worldwide because of their unusual properties and also great potentials for technological applications. Though CNTs continue to attract great interest, other nanotubes such as BN nanotubes (BN-NTs) may offer different opportunities that CNTs cannot provide. In this contribution, we present the results of our recent systematic *ab initio* calculations of the static dielectric constant, electric polarizability, Born dynamical charge, electrostriction coefficient and piezoelectric constant of BN-NTs using the latest crystalline finite electric field theory [1]. [1] I. Souza, J. Iniguez, and D. Vanderbilt, Phys. Rev. Lett. 89, 117602 (2002); P. Umari and A. Pasquarello, Phys. Rev. Lett. 89, 157602 (2002).

> Guang-Yu Guo Department of Physics, National Taiwan University, Taipei 106, Taiwan

Date submitted: 25 Nov 2006

Electronic form version 1.4