

Abstract Submitted  
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**Linear optical response of (6,0) boron nitride nanotubes adsorbed with molecular hydrogen**<sup>1</sup> NORBERTO ARZATE, RAUL A. VAZQUEZ-NAVA, Centro de Investigaciones en Optica, Mexico, JORGE E. MEJIA, Centro Universitario de los Lagos, Universidad de Guadalajara, Mexico — We performed a study of the molecular adsorption of hydrogen on BN nanotubes. We present *ab initio* calculations for the linear optical response of single wall zigzag BN(6,0) nanotubes as a function of the hydrogen adsorption on the exterior surface of the nanotube. The calculation of the linear optical response is performed by using density functional theory with the use of plane waves and pseudopotentials. We consider four different nanotube-structures adsorbed with different coverage of molecular hydrogen. We find optimized atomic coordinates for such structures and calculate binding energies for the molecule of hydrogen on the nanotube. After having the linear response of the considered structures, we have calculated their energy loss function spectra.

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