

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Second-harmonic generation in boron nitride nanotubes adsorbed with molecular hydrogen¹ RAUL VAZQUEZ-NAVA, RAMSES SALAZAR-APARICIO, NORBERTO ARZATE, BERNARDO MENDOZA, Centro de Investigaciones en Optica A. C. — We present *ab initio* calculations for second harmonic response of single wall zigzag pristine and with molecular hydrogen adsorption boron nitride nanotubes. These calculations were performed with density functional theory within the local-density approximation (LDA) and the application of the GW approximation to calculate the band gap GW correction. A length-gauge formalism for calculating the nonlinear optical response with the correct implementation of the scissor correction was used to obtain the nonlinear susceptibility $\chi^{(2)}(-2\omega; \omega, \omega)$ of zigzag BN nanotubes. We found that contrary to that reported in the literature, the (5,0) and (9,0) boron nitride nanotubes have a non vanishing SHG response. We also found that SHG is not a suitable technique to monitor the physisorption of H_2 molecules on the external surface of BN nanotubes.

¹This work was partially supported by CONACYT-México, grants 153930.

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Date submitted: 14 Nov 2013

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