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Effect of Screening on electronic properties of Boron Nitride Nanotube under an electric field in the proximity of a possible metal insulator transition JAY SAU, MARVIN COHEN, UC Berkeley and Lawrence Berkeley National Laboratory — Previous theoretical calculations have shown that the band gap of boron nitride nanotubes can change significantly in a transverse electric field. For large nanotubes it is possible to close the LDA gap with moderately high field strengths. The conduction and valence states in this system are spatially separated creating the possibilty of long-lived excitons. LDA calculations indicate a metallic screening of the field after gap closure. However due to the innately weak screening in Boron Nitride and 1D geometry one can also expect excitonic and other correlation effects to be strong in this system. The screening properties are critical to understanding whether metallic ground state can be reached and whether the possibly long-lived excitons have large binding energies. We estimate the field induced modification of the screening using a tight-binding approach similar to the tight-binding GW/Bethe-Salpeter approach that has previously been used for nanocrystals. The implications of the screening on the possible electronic structures are also examined. This research is supported by National Science Foundation Grant No. DMR-39768, Office of Energy Research, the Office of Basic Energy Sciences and Materials Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. Computational Resources were provided by NPACI and by NERSC.

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