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**Ab initio Bandbending and Schottky Barriers of a Carbon Nanotube and Boron Nitride Device** KHORGOLKHUU ODBADRAKH, PAWEL POMORSKI, CHRISTOPHER ROLAND, North Carolina State University — The quantum transport characteristics of two semiconducting nanotubes (i.e., single-wall (8,0) carbon and boron nitride nanotubes) coupled to metallic leads (i.e., Al (100)) was investigated with a combined nonequilibrium Greens function/density functional theory formalism. The resulting transmission depends very much on the size of the nanotubes: very short tubes are characterized by metallic current-voltage behavior because of transmission via evanescent modes, while longer tubes are dominated by bandbending and Schottky barrier phenomena. An analysis of the latter phenomena as a function of nanotube characteristics, charge transfer, and gate voltage will be presented.

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