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Electronic Transport in B- and N-doped Fullerenes: BC_{59},BC_{60}, NC_{59} and NC_{60} XIAOLIANG ZHONG, RAVINDRA PANDEY, Michigan Tech, Houghton, MI, ALEXANDRE ROCHA, University of São Paulo, São Paulo, Brazil, SHASHI KARNA, US Army Research Laboratory, APG, MD — The electron transport via boron and nitrogen doped fullerenes (i.e. BC_{60}, NC_{60}, BC_{59} and NC_{59}) are studied using first principles methods coupled with non-equilibrium Green's Function formalism. The predicted conductivity for the doped fullerene is higher than that of the pristine fullerene. A substantial conduction is predicted for BC_{59} at higher bias voltage of >1.0 V. The hybrid states near the Fermi region involving contact gold atoms appear to play an important role in determining the conductivity of these systems.

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