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**Charge transport properties of boron/nitrogen binary doped graphene nanoribbons: An ab initio study** SEONG SIK KIM, HAN SEUL KIM, HYO SEOK KIM, YONG-HOON KIM<sup>1</sup>, Graduate School of EEWS, KAIST, YONG-HOON KIM GROUP TEAM — Opening a bandgap by forming graphene nanoribbons (GNRs) and tailoring their properties via doping is a promising direction to achieve graphene-based advanced electronic devices. Applying a first-principles computational approach combining density functional theory (DFT) and DFT-based non-equilibrium Green's function (NEGF) calculation, we herein study the structural, electronic, and charge transport properties of boron-nitrogen binary edge doped GNRs and show that it can achieve novel doping effects that are absent for the single B or N doping. For the armchair GNRs, we find that the B-N edge co-doping almost perfectly recovers the conductance of pristine GNRs. For the zigzag GNRs, it is found to support spatially and energetically spin-polarized currents in the absence of magnetic electrodes or external gate fields: The spin-up (spin-down) currents along the B-N undoped edge and in the valence (conduction) band edge region. This may lead to a novel scheme of graphene band engineering and benefit the design of graphene-based spintronic devices.

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