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Magnetoresistance and negative differential resistance in Ni/Graphene/Ni vertical heterostructures driven by finite bias voltage: A first-principles study¹ KAMAL K. SAHA, University of Delaware, USA, AN-DERS BLOM, QuantumWise A/S, Denmark, KRISTIAN S. THYGESEN, Technical University of Denmark, BRANISLAV K. NIKOLIC, University of Delaware, USA — Using the nonequilibrium Green function formalism combined with density functional theory, we study finite-bias quantum transport in Ni/ Gr_n/Ni vertical heterostructures where n graphene layers are sandwiched between two semi-infinite Ni(111) electrodes. We find that recently predicted pessimistic magnetoresistance of 100% for $n \ge 5$ junctions at zero bias voltage $V_b \to 0$, persists up to $V_b \simeq 0.4$ V, which makes such devices promising for spin-torque-based device applications. In addition, for parallel orientations of the Ni magnetizations, the n = 5 junction exhibits a pronounced negative differential resistance as the bias voltage is increased from $V_b = 0$ V to $V_b \simeq 0.5$ V. We confirm that both of these nonequilibrium transport effects hold for different types of bonding of Gr on the Ni(111) surface while maintaining Bernal stacking between individual Gr layers.

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