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Ab initio study of edge functionalization effects on electronic transport through graphene nanoribbons AMIR FARAJIAN, Wright State University, NARJES GORJIZADEH, YOSHIYUKI KAWAZOE, Tohoku University — We investigate quantum transport through graphene nanoribbons with and without hydrogen saturation. Both armchair-edged and zigzag-edged ribbons with and without hydrogen saturation are considered. For calculating transport properties, we make use of ab initio electronic structure calculations followed by Green's function implementation of the Landauer's formalism. The calculated conductance characteristics show significant dependence on the edge functionalization, i.e., whether or not the armchair and zigzag nanoribbons are saturated by hydrogen atoms. The effects of the carrier spin orientations are also discussed. These results are useful in interpreting the experimental data, and in using functionalized graphene nanoribbons for nanoelectronics and sensor applications.

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