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Polarized Vibrational Infrared Absorption of Graphene Nanoribbons GUANGFU LUO, JING LU, LU WANG, LIN LAI, JING ZHOU, RUI QIN, HONG LI, ZHENGXIANG GAO, State Key Laboratory for Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, People's Republic of China, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182-0266 — In this study, we present the first systematic *ab initio* study of the linearly polarized vibrational IR spectra of the edge-hydrogenated armchair and zigzag GNRs. We reveal that the vibrational IR spectra that provide abundant structural information of GNRs: (1) There is a prominent and width-insensitive IR peak in both GNR types, which can be used as a convenient benchmark in experiment; (2) The major IR absorption of the two GNR types occurs in distinct regions and thus assures a robust feature to distinguish them; (3) In armchair GNRs, the spectra for in-plane polarization oscillate with the ribbon width, while in zigzag GNRs, the dispersion relationship bears close resemblance with that of graphene; (4) One special peak reflecting the mirror symmetry property of zigzag GNRs, which has been proven to be significant in the electronic transport is also discovered; (5) The edge magnetism in zigzag GNRs is found to greatly influence the IR intensity. We expect this work to offer insight into the experimental research and confront the current problem of edge structure identification of GNRs.

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