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Ab initio study of alkali metal adsorption on various forms of graphene nanoribbons SEON-MYEONG CHOI, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology — Electronic and magnetic properties of graphene nanoribbons (GNRs) are very unique depending on their edge shape. While many theoretical studies of GNRs show such intriguing features, clear experimental proofs of atomic edges and their effect on electronic structures have not been explicitly demonstrated. One of the issues is the difficulty of identifying GNRs edges. In this study, we calculated the adsorption energy of alkali metal atoms on various forms of GNRs using the pseudopotential density functional method. We present the distribution of adsorbed atoms on armchair- and zigzag-edged GNRs using the calculated adsorption energy. This approach can help classify the edge of GNRs from the distribution of adsorbed atoms.

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