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Interaction of Lithium and Low-Dimensional Graphene CHANANATE UTHAISAR, JUAN PERALTA, VERONICA BARONE, Central Michigan University — The lithium storage properties of low-dimenstional graphene present a great potential for more efficient rechargeable lithium ion batteries and hydrogen technologies. We study the rich variety of electronic and magnetic properties of graphene nanoribbons with two different edges, zigzag and armchair, by using density functional theory. We found that Li adsorption is stronger in zigzag nanoribbons than in two-dimensional graphene, fullerene and armchair nanoribbon. The strongest binding occurs when the Li-atom is located at the edge of zigzag nanoribbons. The evaluation of Li diffusion coefficient on the surfaces of graphene nanoribbons will be discussed. We will also show that the enhanced Li-zigzag nanoribbon interaction affects significantly their magnetic properties by quenching the magnetization in the areas neighboring the absorption site. Moreover, based in our first-principles calculations, we will report their Li intake capacity and rationalize it in terms of their peculiar properties and morphology.

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