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**Two-dimensional Arsenene as a potential anode material for LIBs, NIBs or MIBs: First principal study**

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In view of the interest in new energy storage technologies. A novel architecture using two dimensional (2D) nanomaterials have been widely attracted researcher for designing a new electrode material with nanometer improving the performance of lithium-ion batteries, including Na-ion batteries, Mg-ion batteries In this paper, the first-principles density Arsenene likely to phosphorene are atomic thick material, it is possible to be manufactured in experiment by exfoliating from grey due to the weak interaction between layers of grey arsenic. Functional theory (DFT) calculations are employed to investigate and compare the interaction of Na, Mg and Li ions with arsenene monolayer. The results indicate that the Li, Na and Mg adatom preferably adsorbed on valley sites, with negative adsorption energy of -2.55, -1.91 and -1.10 eV, respectively. Then the ions concentration increased until the full saturation of the surfaces is achieved. The highest capacity estimated to be 358 mA h g<sup>-1</sup> which is close to graphite and phosphorene capacity. Accordingly, a semiconductor to conductor transition is observed and gives rise to a good electrical conductivity. Furthermore, the diffusion barrier energies of Li, Na and Mg ions are calculated using utilized nudged elastic band method. The activation energy barriers of these ions show isotropic behavior for different pathway (X, Y and diagonal direction) where the obtained values are 0.16, 0.05 and 0.016 eV, for Li, Na and Mg ion, respectively. Our findings show that the high capacity, low open circuit voltage, ultrahigh barrier diffusion makes the arsenene a good candidate for application as an electrode material for Li (Na or Mg) batteries.

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