



Mn₂C sheet as an electrode material for lithium-ion battery: A first-principles prediction



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ABSTRACT

A search for high-efficiency electrode materials is crucial for the application of Li-ion batteries (LIBs). Using density functional theory (DFT), we assess the Mn₂C sheet, a new MXene, as a suitable electrode material. Our studies show that Li atoms can bind strongly to the Mn₂C sheet, with low adsorption energy of -1.93 eV. A pristine Mn₂C sheet exhibits metallic characteristic, offering an intrinsic advantage for the transportation of electrons in material. A very low energy barrier of 0.05 eV is predicted, showing that Li ion can easily and freely migrate on the Mn₂C sheet. In addition, with the increase of Li content, adsorption energy varies minimally within a range of energy that spans only 0.27 eV, showing that lithiation to a high content is feasible. Furthermore, we found that, because of the bilayer adsorptions on both sides of the Mn₂C sheet, the theoretical capacity of the Mn₂C sheet is 879 mAhg⁻¹, which is greater than that of most two-dimensional (2D) electrode materials. All these results reveal a new promising MXene material for LIBs. We also studied the effects of oxidation and fluorination on the electrochemical properties of the Mn₂C sheet and found that oxidation and fluorination will fade the electrochemical properties of the Mn₂C sheet in general.

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1. Introduction

Research on advanced energy storage technology is essential for the development of modern society [1,2]. The LIB, one of the most widely studied rechargeable batteries, is believed to be the best choice for energy-efficient and environmentally friendly energy storage technology [3–5]. Currently, LIBs are widely used in portable electronics, electric vehicles, and electricity grid systems [6,7]. Nevertheless, they still do not satisfy the requirements of the modern electronics market, with high energy storage density, high rate capacity, good cycling stability, and low cost. Note that the performance of LIBs is highly dependent on the properties of the electrode materials [8,9]. Consequently, the development of novel and efficient electrode materials becomes a key challenge for the next generation of renewable energy technologies.

2D materials are of special interest as electrode materials for LIBs because of their huge surface-to-volume ratio, which enables fast ion diffusion and large ion capacity. The growing interest in 2D layered structures greatly accelerated the development of LIBs in

recent years [10,11]. Graphene represents the first example of a 2D electrode material for LIBs [12,13]. However, the results of Li storage performance using pristine graphene are rather controversial that some studies suggested that graphene can provide large reversible capacity, superior rate capability, and long cycle life [14,15], while others concluded that Li adsorption on graphene is rather difficult due to the repulsiveness of adjacent Li ions and the formation of Li clusterings [16,17]. Since then, layered MoS₂ has attracted a great deal of attention. While MoS₂ possesses intrinsic fast ionic diffusion and high theoretical capacity [18–20], the poor electronic transportation capability, thermal instability, and significant volume change still impede its application [21]. Thus far, the possibilities of using novel 2D structures, such as silicene [22,23], graphyne [24–27], phosphorene [28,29], borophene [30], VS₂ sheet [31], Mo₂C sheet [32,33], BSi₃ sheet [34], GeS sheet [35], and transition-metal oxide sheets [36,37], for Li storage have been explored. Although these novel 2D structures have been confirmed as potential electrode materials with high capacity, low diffusion barrier, and superior electronic conductivity theoretically, high-yield, simple, and mass production of these structures experimentally, which is critical for their widescale use, is still a challenge. Bearing this in mind, the search for new promising 2D electrode materials for next-generation LIBs is still essential.

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2D transition metal carbides or nitrides, called MXenes, recently attracted much attention [38,39]. MXenes can be viewed as the 2D counterpart of MAX phase of $M_{n+1}AX_n$ type, where M and A are transition metal and main group elements, respectively, and X is C and/or N. In MAX phase, compared with the MX layer with exceptionally strong M–X bonds, the A-containing plane layer is relatively weakly bonded. Thus, by immersing $M_{n+1}AX_n$ powders into hydrofluoric acid, it is extremely easy to successfully fabricate a mass of exfoliated and separated MXenes experimentally, offering an intrinsic potential for their practical applications [40–44]. Some studies for MXenes, mainly focused on Ti_2C and Ti_3C_2 sheets, have been carried out in previous works [45–48]. For example, Mashtalir et al. reported that delaminated Ti_3C_2 can have a Li capacity of up to 410 mAhg^{-1} , combined with good rate capability [49]. Subsequent experimental studies further demonstrated that Li capacities of MXenes can be enormously improved by H_2O_2 treatment or heat treatment [50,51]. Theoretically, Tang et al. and Er et al. predicted that pristine transition-metal carbides, specially Ti_2C and Ti_3C_2 sheets, can possess superior electrical conductivity, low diffusion barrier, and high theoretical capacity [52,53]. Subsequent theoretical studies further confirmed that the storage capacities of transition-metal carbides can be drastically

boosted by functionalizing the M atom of MXene by the O atom [54,55]. While some investigations have been conducted, MXene electrode materials with solid performance are still under development.

Herein, we studied the interaction of Li with the Mn_2C sheet, a new MXene, by means of DFT. Mn_2C sheet here can be viewed as a 2D counterpart of the recently synthesized Mn_2GaC compound [56]. A practical process is to explore another new promising MXene electrode material for LIB. This paper is organized as follows: (i) we first optimized the structure of Mn_2C sheet; (ii) we then investigated the electrical conductivity of Mn_2C sheet based on the analyses of total and projected density of states (DOS); (iii) next, we determined the most favorable adsorption site of Li on Mn_2C sheet by comparing the adsorption energies of Li at different sites; (iv) we then examined the diffusion barriers of Li on Mn_2C sheet in order to evaluate the potential of Mn_2C sheets as high-rate electrode material; (v) we obtained the most stable adsorption structures of lithiated Mn_2C sheets with increasing Li content and calculated corresponding adsorption energies; (vi) finally, we predicted a specific capacity of Mn_2C sheets based on the maximal Li adsorption content; (vii) in addition, we studied the effects of oxidation and fluorination on the electrochemical behaviors of

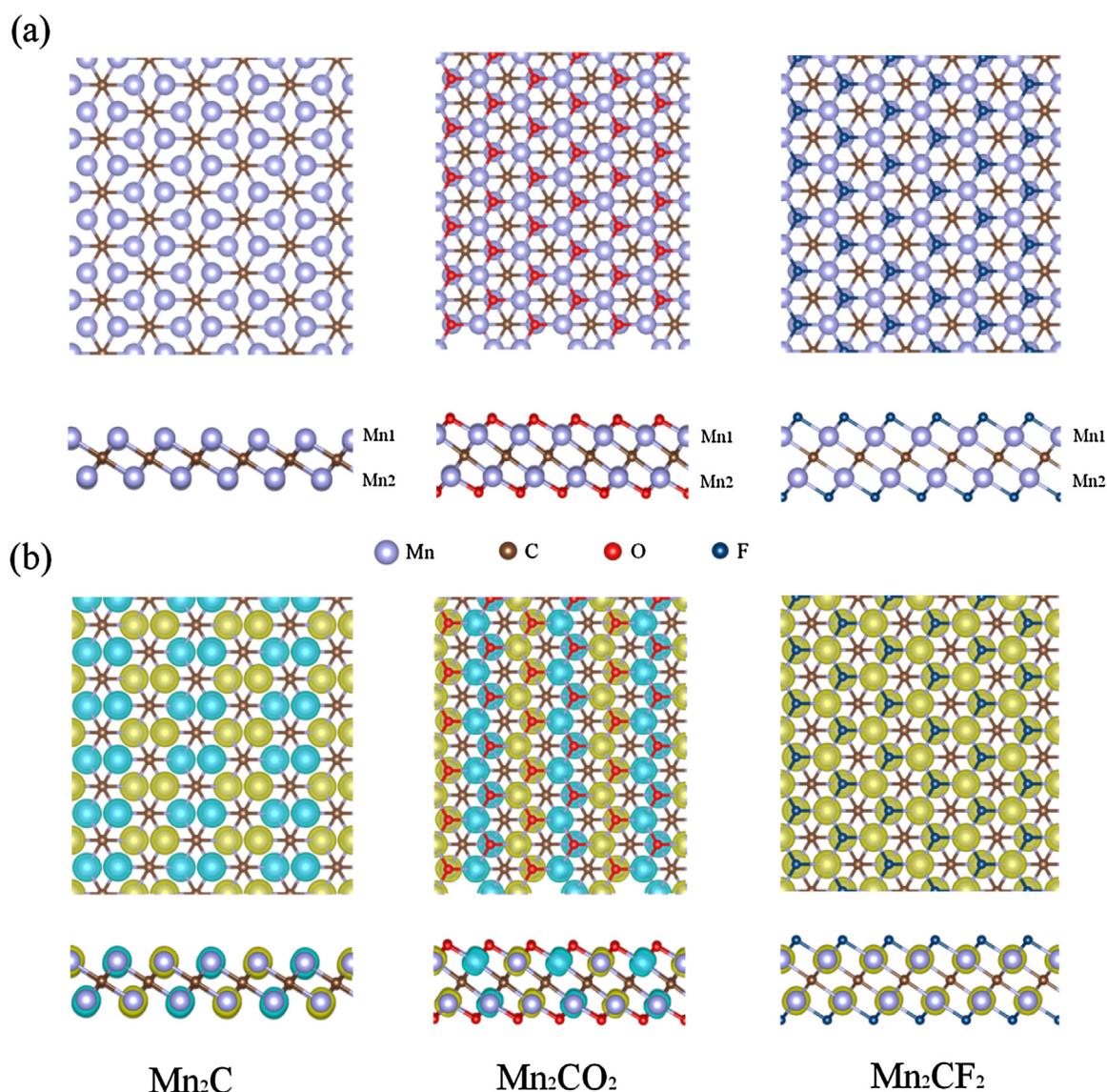


Fig. 1. (a) Geometries and (b) spin ground states of the most stable Mn_2C and Mn_2CX_2 ($X=O, F$) sheets.

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