A high-performance anode material based on FeMnO₃/graphene composite

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Abstract: Transition metal oxides are attractive as anode materials in lithium-ion batteries for their high theoretical capacity and good performance. In this work, an anode material based on manganese-based oxide FeMnO₃ in LIBs is investigated for the first time. FeMnO₃ is prepared with graphene and the FeMnO₃/graphene composite exhibits a high discharge capacity of 1155.3 mAh g⁻¹ after 300 cycles at 200 mA g⁻¹, as well as a superior rate performance of 851.7 mAh g⁻¹ at a current density of 3200 mA g⁻¹. The observed extraordinary performance is believed to be attributed to the combination of the intrinsically high capacity of FeMnO₃, a large surface area of 89.65 m² g⁻¹ and good electrical conductivity of the FeMnO₃/graphene composite. To help clarify the properties of this new material, we employ first principles calculations to determine the structural stability, electronic structure, and Li

ion diffusivity of FeMnO_3 . The calculations show that FeMnO_3 has a relatively low band gap (an indication of reasonable electrical conductivity) and Li ions exhibit a large room temperature diffusivity in FeMnO_3 .

Keywords: manganese-based oxide, anode, graphene, Li-ion battery, first principles calculations.

1. Introduction

With the rapid development of portable electronic devices and hybrid-electric vehicles, lithium-ion batteries (LIBs) are becoming more and more attractive, due to their high energy density, fast charge/discharge rate and long cycling life [1-3]. Unfortunately, the low theoretical capacity of 372 mAh g^{-1} of commercial graphite anodes is a limit on the overall energy density of the cell. Significant effort has been made in searching for potential substitutes for graphite as the anode material. Transitional metal oxides [4,5], including zinc oxides [6], manganese oxides [7-10], iron oxides [11,12], cobalt oxides [13], and tin oxides [14] have demonstrated excellent properties as anode materials in LIBs. Among them, manganese oxides and related compounds have attracted particular attention. They possess not only high energy capacity and low conversion potential but also some other advantages such as multiple valence states, earth-abundant elements, low toxicity and cost. For example, Mn_2O_3 with diverse morphologies has been reported to show a reversible discharge capacity of 470.3 mAh g^{-1} at a current density of 3200 mA g^{-1} after 100 cycles [8]. Generally speaking, metal oxides have poor electrical conductivity, but this can be improved by doping with other elements [15,16]. Therefore the manganese-based ternary oxides may have better performance in LIBs compared with manganese

oxides. Bijelić et al. [17] reported that the manganese-based ternary oxide, CoMn_2O_4 , has a long cycle life with a capacity of 624 mAh g^{-1} after 1000 cycles at 200 mA g^{-1} .

Here, we turn our attention to another manganese-based oxide, FeMnO_3 , which has previously attracted more attention due to its magnetic properties [18] than its electrochemical properties. FeMnO_3 has a bixbyite crystal structure with Fe and Mn ions randomly occupying the 8b and 24d sites with an atom ratio of 1:1 [19]. Here, we demonstrate the synthesis and the performance of FeMnO_3 as an anode in LIBs. Furthermore, by combining oxides with active carbon materials in various nanostructural morphologies, one can enhance the electrochemical reaction kinetics and performance [12,20]. For instance, graphene has been used to buffer volume change, anchor active materials and prevent nanostructural oxides from agglomerating during continuous charge/discharge cycles in LIBs [21-23]. Therefore graphene is a good candidate for the FeMnO_3 composite because it has large specific surface area and high electron conductivity.

Herein, a two-step procedure was established for the synthesis of a FeMnO_3 /graphene composite. When the prepared composite used as an anode in LIBs, it shows very favorable electrochemical properties: a high reversible capacity of $1155.3 \text{ mAh g}^{-1}$ after 300 cycles at 200 mA g^{-1} and a good rate performance of 851.7 mAh g^{-1} at a current density of 3200 mA g^{-1} . The electrical conductivity of the FeMnO_3 and the diffusivity of Li ion in FeMnO_3 were also calculated by using density functional theory (DFT). In the calculations, the Special Quasi-random Structure (SQS) [24] method and ab-initio molecular dynamic simulations were used to determine the disordered structure of FeMnO_3 , predict the band gap of the disordered bixbyite compound, and determine the temperature-dependent Li ion diffusivity in FeMnO_3 . The calculations show that FeMnO_3 is a low-bandgap

semiconductor, with a small band gap of ~ 0.3 eV (Silicon, 0.75 eV [25]), and the diffusivity of Li ion in FeMnO_3 is $\sim 3.9 \times 10^{-12} \text{ cm}^2 \text{ s}^{-1}$ which is comparable to state-of-the-art fast Li-ion conducting electrode materials (LiMn_2O_4 , $\sim 10^{-11} \text{ cm}^2 \text{ s}^{-1}$ [26] and graphite, $1.12 \times 10^{-10} \text{ cm}^2 \text{ s}^{-1}$ [27]).

2. Experimental

2.1 Synthesis of FeMnO_3 and graphene composites

FeMnO_3 /graphene composite (denoted as FMO-RGO) was synthesized via a two-step procedure. In the first step, 5 mmol of $\text{Mn}(\text{COOCH}_3)_2 \cdot 4\text{H}_2\text{O}$ and 5 mmol of $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ were dissolved in 20 mL of deionized water under 0.5 h magnetic stirring at room temperature. Then 0.5 mL of ammonia solution was added into the above solution drop by drop under continuously magnetic stirring for 0.5 h which resulted in a brown suspended solution. The brown suspension was collected by centrifugation and washed with deionized water three times before dried at 60°C for 12 h. Subsequently, the dried product was calcined at 550°C for 3 h in air and FeMnO_3 particles were obtained (denoted as FMO). In the second step, graphene oxide (GO) was prepared from natural graphite flakes using a modified Hummers method. Then 40 mg of the obtained FMO and 17 mg of GO were added into 20 mL of deionized water and the solution was under ultra-sonication treatment for 0.5 h. Afterward, the solution was transferred into a 60 ml Teflon-lined stainless steel autoclave which was heated at 180°C in an oven for 3 h and then furnace cooled to room temperature. Finally the obtained product was collected through centrifugation, washed with deionized water three times and dried at 60°C for 6 h in an oven. For a comparison, GO was reduced to RGO in the same hydrothermal process at 180°C in an oven for 3 h but without the presence of FMO. Then FMO was physically mixed with RGO also

at the mass ratio of 7:3 and the mixture is denoted as FMO/RGO MIX. In this investigation the electrochemical performance of the bare FMO was also conducted as a reference.

2.2 Characterization

The obtained samples were characterized by X-ray powder diffraction (XRD) on a RigakuD/max 2550VL/PC system operated at 35 kV and 200 mA with Cu K α radiation ($\lambda = 1.5406 \text{ \AA}$). The atomic ratio of Fe and Mn in FMO was analyzed by using X-ray fluorescence spectrometer (XRF, EDX-720). X-ray photoelectron spectroscopy (XPS) was carried on a physical electronics PHI5400 using Mg K α radiation as the X-ray source. Raman spectroscopy was performed on a SENTERRA R200 Raman microscope. All the spectra were corrected with C 1s (284.8 eV) band. Nitrogen adsorptions at 77 K were measured on an ASAP2020 volumetric adsorption analyzer. Scanning electron microscopy (SEM) was performed on a JEOLJSM-6360LV field emission microscope at 15 kV. Transmission electron microscopy (TEM) was carried out on a JEOL2010 microscope at 200 kV.

2.3 Electrochemical measurement

Electrochemical experiments were performed on coin-type cells which were assembled in an argon filled glove box (Mikrouna1220/750). The working electrodes were made by mixing the FeMnO₃/graphene composite with carbon black and a binder (polyvinylidene fluoride, PVDF) at a mass ratio of 8 : 1 : 1. The mixture was cast on copper foils of 12 mm in diameter and dried in vacuum at 110 °C for 12 h. A typical loading mass of the active material was 0.8-1.2 mg. Metallic lithium foil was used as the counter electrode and Celgard 2300 microporous membrane was used as

the separator. The electrolyte was made of 1 M LiPF₆ dissolved in the mixture of ethylene carbonate (EC) and diethylene carbonate (DEC) with the volume ratio of 1 : 1. The galvanostatic charge/discharge experiment was carried on a Land CT2001A battery test system in the potential range of 0.01–3.0 V at 25±3°C. Cyclic voltammetry (CV) curves were acquired on a Chenhua CHI 660D electrochemical workstation in the potential range of 0.01–3.0 V at a scan rate of 0.5 mV s⁻¹. Electrochemical impedance spectroscopy (EIS) was carried out on a Chenhua CHI 660D electrochemical workstation with an AC voltage 5 mV, in the frequencies between 100 kHz and 0.01 Hz. For comparison, the electrochemical performances of the FMO and FMO/RGO MIX electrodes were measured under the same condition.

2.4 Computational Methodology

2.4.1 Density functional theory calculations

The first principle calculations were conducted using the Vienna Ab-initio Simulation Package (VASP) [28-31] and the projector augmented wave (PAW) potentials [32]. The generalized gradient approximation (GGA) of Perdew-Becke-Ernzerhof (PBE) [33] was used for the exchange-correlation function. In all calculations FeMnO₃ is assumed to be ferromagnetic (FM) and spin polarized though FeMnO₃ is known to display antiferromagnetic (AFM) ground states at around 39 K [18,19]. The AFM state is observed well below room temperature, so we assume that the energetic effect of magnetic ordering is small, and the approximation of a FM configuration should not result in significant error. A plane-wave basis set with a cutoff energy of 520 eV and Γ -centered k -meshes with an approximate density of 8000 k -points per reciprocal atom were used in all calculations. The DFT+ U method was used to treat Fe-3d ($U_{Fe} = 4.0$ eV) and Mn-3d ($U_{Mn} = 3.8$ eV) states following the

previous work [34-36]. In the bixbyite structure of FeMnO_3 , Fe and Mn ions form fcc arrays and O occupies 3/4 of the tetrahedral sites and all octahedral sites are unoccupied. The unit cell of Mn_2O_3 bixbyite structure has 32 metal sites (80 atoms). We populate these metal sites with Fe and Mn equally and randomly and construct the computational unit cell using the special quasi-random structure (SQS) method. An SQS was generated based on a Monte Carlo algorithm implemented in ATAT [37-47] with the constraint that the pair and triplet correlation functions of the SQS are identical to those of the statistically random Fe/Mn population of cation sites at least up to the third nearest neighbor.

2.4.2 *The room temperature diffusivity evaluation by ab-initio molecular dynamic (MD) simulations*

In order to evaluate the Li ion diffusivity in FeMnO_3 , we performed ab-initio molecular dynamics (MD) simulations in VASP using the SQS structure of FeMnO_3 consisting of 16 f.u. and a dilute amount of Li. A minimal Γ -centered $1 \times 1 \times 1$ k-point grid was chosen to keep the computational cost at a reasonable level after a convergence test. Our simulations were performed in the canonical ensemble using the Nose thermostat [48,49]. For each run, we used the Velocity-Verlet time integration scheme with a time step of 2 femtoseconds. To account for thermal expansion, the supercell volume was determined for each temperature by the volume where the average pressure was approximately zero based on a series of short (1 picosecond) runs at varying volumes [50]. In the MD simulations, the FeMnO_3 compound was assigned an initial temperature of 100 K. Then the system was heated up to target temperatures (600 K to 1800 K) in 2 picoseconds and equilibrated for 5 picoseconds. The MD simulations for the diffusion were then performed for 40

picoseconds with no sign of melting [51]. The diffusivity of each target temperature was obtained by fitting the mean square displacement over time:

$$D = \frac{1}{2t} \langle [r(t)]^2 \rangle \quad (1)$$

where $r(t)$ is the displacement of Li ions at time (t). D is obtained by a linear fitting to the dependence of average mean square displacement over $2t$. The room temperature diffusivity was obtained by extrapolating the diffusivity values at target temperatures to room temperature based on the Arrhenius relationship. When the diffusivity values at different temperatures were collected, the activation barrier is evaluated by linear fitting of the slope of the diffusivity profile versus $1/T$:

$$\ln(D) = \ln(D_0) - E_{Act}/kT \quad (2)$$

where D_0 is the temperature-independent pre-exponential. E_{Act} is the activation barrier. k is the Boltzmann constant.

3. Results and discussion

The FeMnO₃/graphene composite (FMO-RGO) and pure FeMnO₃ (FMO) were characterized by X-ray diffraction and the results are given in **Fig. 1**. The diffraction peaks located at $2\theta = 23.1^\circ$, 33.0° , 38.2° , 55.2° and 65.7° are indexed as cubic FeMnO₃ (JCPDS card No.75-0849), without any signs of other impurity phases. The XRD diffraction patterns of FMO and FMO-RGO are virtually identical. It is worth mentioning that FeMnO₃ (JCPDS card No.75-0849) and α -Mn₂O₃ (JCPDS card No.71-0636) have the nearly same diffraction pattern (**Fig. 1**). Therefore FeMnO₃ has the same crystal structure as α -Mn₂O₃. That means half of the manganese atoms in α -Mn₂O₃ are substituted by iron atoms in FeMnO₃ without changing the crystal structure. [The analysis of X-ray fluorescence spectrometer \(XRF\) find that the atomic](#)

ratio of Fe and Mn in FMO is 1.03 : 1 ($\approx 1 : 1$), further confirming the successful synthesis of FMO.

X-ray photoelectron spectroscopy (XPS) was performed to characterize the elemental composition and bonding configuration of FMO-RGO. **Fig. 2a** shows the spectrum of Fe 2p with two large peaks located at 724.6 eV (Fe 2P_{1/2}) and 711.2 eV (Fe 2P_{3/2}). The two minor satellite peaks next to the large peaks are due to the existence of Fe³⁺ [52]. In **Fig. 2b**, two characteristic peaks of Mn 2p located at 653.3 eV (Mn 2P_{1/2}) and 641.6 eV (Mn 2P_{3/2}) are attributed to Mn³⁺ [53] with no sign of other valence states of the manganese ions. This result is also consistent with the XRD analysis that FeMnO₃ was successfully synthesized (**Fig. 1**).

Raman spectroscopy was used for the characterization of graphene in FMO-RGO and the results are shown in **Fig. 3**. The two peaks at 1350 and 1590 cm⁻¹, correspond to the well-defined D band and G band of RGO, respectively. The low D/G intensity ratio ($I_D/I_G < 1$) illustrates the formation of reduced graphene oxides during the hydrothermal treatment. Two small peaks at 312 and 653 cm⁻¹ are attributed to the presence of FeMnO₃ in FMO-RGO [54].

The pore size and surface area of the electrode materials were measured by using nitrogen adsorption–desorption isotherms (**Figs. 4**). The specific surface area of FMO-RGO calculated from BET is 89.65 m² g⁻¹ which is more than twice the value (39.23 m² g⁻¹) of FMO. The average pore size of FMO (**inset of Fig. 4a**) is calculated to be 16 nm using the Barrett–Joyner–Halenda (BJH) method. This type of pores is likely resulted from the aggregation of FMO particles. In FMO-RGO, in addition to the 16nm pores, there is a distinct new type of mesopores centered at 4 nm which are possibly formed between the FMO particles and reduced graphene sheets.

From SEM images, it is apparent that FMO consists of particles with a variety of sizes and shapes (**Fig. 5a**). A high magnification image shown in **Fig. 5b** reveals that the FMO particles are made of small particles. **Figs. 5c** and **d** show that the microstructure of FMO-RGO which consists of FeMnO_3 particles and graphene. In comparison with the FMO sample, graphene sheets are observed with FMO particles anchored on them (**Fig. 5d**). Further analysis of the TEM image in **Fig. 5e** reveals that the FMO particles approximately 30-40 nm in diameter are homogeneously dispersed on the surface of graphene sheets. A high resolution TEM image of a single primary particle (**Fig. 5f**) shows the lattice fringes of the (222) plane of FeMnO_3 , revealing the highly crystalline nature of FMO/RGO, which is confirmed by the analysis of SAED pattern shown in the inset of **Fig. 5f**.

Cyclic-voltammetric measurements were carried out to assess the electrochemical properties of the sample FMO-RGO (**Fig. 6a**). In the first cathodic sweep, two peaks are detected at around 0.55 and 1.1 V respectively. The tiny peak at 1.1 V is attributed to the reduction of Mn^{3+} to Mn^{2+} [17,55], which disappears in subsequent cycles. The sharp peak at around 0.55 V is assigned to the reduction reactions of Mn^{2+} and Fe^{3+} to their metallic states embedded in the Li_2O structure [17,55,56], which shifts at around 0.7 V in the second and third cycles. A peak attributed to the formation of a solid electrolyte interphase layer (SEI) in manganese-based oxide electrode usually at from 0.7 to 0.9 V [55,57] was not observed. It is possible that the sharp peak at 0.55 V obscured the SEI peak at adjacent voltage. In the first anodic sweep, the broad peaks at around 1.3 and 1.75 V are attributed to the oxidation reactions of Mn to MnO and Fe to Fe_3O_4 , respectively [17,55,56]. In the second and third anodic sweeps, there is little change in the oxidation reaction of Mn^0 to Mn^{2+} at the peak at 1.3 V but slight changes in the oxidation reaction of Fe to Fe_3O_4 at the peak from 1.75 to 1.85 V.

Moreover, a new peak appears at around 2.1 V and it becomes strong during the discharge/charge process, indicating the occurrence of higher oxidation state of Mn [21].

The galvanostatic charge/discharge experiments were conducted to evaluate electrochemical properties of LIBs and the results are shown in **Fig. 6b**. The FMO-RGO based electrode shows a specific capacity of 1569.2 mAh g⁻¹ in the first cycle at a current density of 200 mA g⁻¹. The electrode still displays a very high capacity of 1008.8 mAh g⁻¹ even in the 100th cycles. The FMO based electrode displays a specific capacity of 1021 mAh g⁻¹ in the first cycle and it decreases very quickly to only 127.4 mAh g⁻¹ in the 100th cycles. This value is much lower than 1008.8 mAh g⁻¹ of FMO-RGO. In order to understand the role of graphene, the electrochemical performance of mechanically mixed FMO and RGO: FMO/RGO MIX, was measured and the results are shown in **Fig. 6b**. The FMO/RGO MIX electrode displays a specific capacity of 1183.4 mAh g⁻¹ in the first cycle and then the capacity decreases to 432.6 mAh g⁻¹ in the 100th cycles. Although it is much higher than the 127.4 mAh g⁻¹ of the pure FMO, the 432.6 mAh g⁻¹ capacity of FMO/RGO MIX is much lower than 1008.8 mAh g⁻¹ of FMO-RGO. That implies that some interfacial interactions between the FMO and RGO occurred in FMO-RGO but not in FMO/RGO MIX. Further investigation on FMO-RGO found that a specific capacity of 1155.3 mAh g⁻¹ can be retained even after 300 cycles (**Fig. 6c**), indicating a superior reversible capacity of FMO-RGO compared to that of the previously reported transition-metal oxides such as Mn₂O₃ [8], Mn₃O₄ [9] and CoMn₂O₄ [15]. This good reversible capacity of FMO-RGO likely results from a combined effect of the high theoretical capacity storage of FeMnO₃ and the limited aggregation of active materials (since they are anchored on the graphene sheets). It is worth noting that the specific

capacity increases in two stages in **Fig. 6c**. The increase associated with the first stage which is from 60 to 130 cycles, possibly is due to the activation process of the anode materials [55,58], and the second stage increase which begins at the 180th cycle, is probably due to the valence of manganese changes from Mn^{2+} to higher than Mn^{2+} as illustrated by others [21,59]. Moreover, the composite shows an exceptional rate performance as it can be seen that an extremely high capacity of 851.7 mAh g^{-1} at a current density of 3200 mA g^{-1} is achieved (**Fig. 6d**). When the current density increases from 200 mA g^{-1} to 3200 mA g^{-1} and then returns to 200 mA g^{-1} , FMO-RGO exhibits a stable capacity recovery at 1190 mAh g^{-1} and this capacity is retained upon the subsequent cycles.

Electrochemical impedance spectroscopy (EIS) plots of FMO-RGO and FMO based electrodes in the initial state and the 10th cycle state are compared in **Figs. 7a** and **b**. The semicircles in the high- and medium-frequency regions are representative of the solid electrolyte interface (SEI) resistance and the charge-transfer impedance, respectively [59]. The impedance of the FMO-RGO based electrode is much smaller than that of the FMO electrode both in the initial state and the 10th cycle, therefore FMO-RGO has better electrical conductivity than the pure FeMnO_3 . Moreover, the impedance of FMO-RGO is stable during the charge/discharge process, which is possibly attributed to that the graphene prevents the FeMnO_3 particles from aggregating, but the impedance of FMO increases greatly after 10 cycles.

In an effort to further understand the properties of FMO, we use first-principles DFT calculations to predict the band gap and Li ion diffusivity of FMO. The quasi-random (SQS) structure of FMO used for the calculation is shown in **Fig. 8a** and **Table S1**. The DFT calculations show that the band structure of the FMO has "half semiconductor" features: a very small gap in one spin channel and a relatively

large gap in the opposite spin channel. The small band gap around 0.3 eV (Silicon, 0.75 eV [25]) of FMO suggests it might have a good electrical conductivity (**Fig. 8b**). **Fig. 8c** shows the Arrhenius plot for the calculated diffusion coefficients at temperatures from 600 K to 1800 K. The extrapolated Li ion diffusion coefficient of FMO at room temperature is $3.9 \times 10^{-12} \text{ cm}^2 \text{ s}^{-1}$ with an activation energy of 0.51 eV (**Fig. 8c**) which is comparable to most state-of-the-art high-rate electrode materials like LiMn_2O_4 , $\sim 10^{-11} \text{ cm}^2 \text{ s}^{-1}$ [26] and graphite, $1.12 \times 10^{-10} \text{ cm}^2 \text{ s}^{-1}$ [27]. The calculated small band gap and high Li ion diffusivities lead to the high kinetics in the lithiation reaction and fast diffusion channels for lithium ions, which are beneficial to the performance of FMO based electrode in LIBs as reported in other materials [60]. A high specific capacity of 1021 mAh g^{-1} of the FMO based electrode in the first cycle is consistent with this calculation. As a composite electrode material of FMO-RGO, adding graphene properly to transition metal oxide electrode material can enhance corresponding capacities and ionic conductivities by offering larger surface area and shorter Li transport path length, as evidenced by the results.

4. Conclusions

In summary, we successfully prepared FeMnO_3 and measured its electrochemical properties. To enhance the electrochemical performance of FeMnO_3 , graphene was introduced to make a $\text{FeMnO}_3/\text{graphene}$ composite. The resultant composite exhibited a high reversible capacity of $1155.3 \text{ mAh g}^{-1}$ after 300 cycles at 200 mA g^{-1} , as well as a very good rate performance of 851.7 mAh g^{-1} at a current density of 3200 mA g^{-1} . This high performance is believed to be attributed to intrinsically high capacity of FeMnO_3 , a large surface area of $89.65 \text{ m}^2 \text{ g}^{-1}$ and good electrical conductivity of the $\text{FeMnO}_3/\text{graphene}$ composite. In other words, the excellent performance is due to the

synergy between the intrinsic FeMnO_3 and the graphene sheets. Furthermore, the DFT calculations showed that FeMnO_3 has a small band gap (indicating the possibility of good electrical conductivity) and excellent Li ion diffusivity in FeMnO_3 . These properties are important for an electrode. The high-performance anode material based on the FeMnO_3 /graphene composite reported here provides us a promising anode material for LIBs.

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Figure captions:

Fig. 1. XRD patterns of samples FMO and FMO-RGO.

Fig. 2. (a) Fe 2p and (b) Mn 2p survey XPS spectra of FMO-RGO.

Fig. 3. Raman patterns of FMO-RGO.

Fig. 4. N₂ absorption/desorption isotherm plot of (a) FMO and (b) FMO-RGO (pore diameter distribution curve (inset)).

Fig. 5. SEM images of (a), (b) FMO and (c), (d) FMO-RGO. (e) TEM, (f) HRTEM and SAED (inset (f)) images of FMO-RGO.

Fig. 6. (a) Cyclic-voltammograms of FMO-RGO at a scan rate of 0.5 mV s⁻¹. (b) Cycling performance of FMO-RGO, FMO/RGO MIX and FMO at a current density of 200 mA g⁻¹. (c) Cycling performance of FMO-RGO at a current density of 200 mA g⁻¹ for 300 cycles. (d) Rate performance of FMO-RGO at various current densities.

Fig. 7. (a) Initial state and (b) 10th cycle at a current density of 500 mA g⁻¹ EIS results of FMO-RGO and FMO based electrode.

Fig. 8. (a) The disordered structure of the FeMnO₃ generated by the SQS method. (b) Calculated density of states for the FeMnO₃. (c) Arrhenius plot of the Li ion diffusion coefficient in FeMnO₃. The error bar corresponds to statistical uncertainty in the fitting of the mean square displacement to time curve.

Figures:

Figure 1

Figure 2

Figure 3

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Figure 8