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NANOSTRUCTURED MOS_2 FOR ENERGY STORAGE (SUPERCAPACITORS): A REVIEW

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ABSTRACT

High efficiency energy storage devices are one of the greatest scientific and engineering challenges to power the various electronic equipment of the twenty first century and this instigated research on innovative energy storage devices. Recently, transition metal chalcogenides, specifically molybdenum chalcogenides, have get great attention of the researchers due to their amazing physicochemical as well as mechanical properties. Owing to its high anisotropy and distinct crystal structure, numerous reports indicates that nanostructured MoS_2, with the merits of low cost and prominent properties, is an excellent substitute for environmentally benign energy conversion and for use in storage devices like supercapacitors. In this paper, detailed review has been done on the effects of impurities and defects on MoS_2 by ab-initio density functional theory (DFT) and molecular dynamics. We have also reviewed the possibilities of realizing magnetic nanostructures, trapped at the vacancy defects in MoS_2.

Keywords:*MoS_2, Molecular dynamics, DFT, Supercapacitors*

Introduction

New era of technology is leading us towards unconventional, clean energy as well as more compact, smaller and durable devices. Fossil fuels were the major source of energy for last few centuries, but it was not a renewable source of energy [1,2]. A series of environmental issues have been emerging since last century as a result of the very high consumption of fossil fuels. Supercapacitors are the latest energy storage devices also called ultra-capacitors or electrochemical capacitors, which are designed to bridge the gap between batteries and capacitors to form fast charging energy storage devices to support intermediate [5].

Ab initio density functionaltheory

The first principles methods or ab initio methods consider electrons as the fundamental particles and explains the event in a subatomic world. So the system in ab initio method can only be expressed by quantum mechanics. The calculation methods in this method are based on only quantum mechanics, so there is not any use

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of fitting parameters from any experimental data, which is generally occur in molecular dynamics. Quantum mechanics involves relatively difficult partial differential equations. All the calculations are solely based on the basic laws of physics [14]. Till the 3rd decade of 20th century, only simple atoms like hydrogen were simulated by quantum mechanical simulations, but now the number of atoms has reached to over several thousand by the arrival of density functional theory (DFT).

Molecular dynamic ssimulation

Molecular dynamics take into account atoms as the smallest unit (basic particles) of the material. MD disregards nuclei (Protons + Neutrons) and electrons [14]. Therefore, any system can be easily described by using Newton's classical equations of motion that is considerably easy as it has only atom to atom interactions. In 6th decade of 20th century, only hundreds of atoms were simulated by using MD simulation techniques. But now the number of atoms has increased to over 100 billion till date. The only problem with MD simulation is that we have to empirically generate the potential file (interacting potential among the atoms) as origin of nuclei and electrons are completely ignored in this method. So that magnetic properties as well as electronic properties can't be obtained [17].

Applications Of Supercapacitors:

As It is a new kind of energy storage device, it has a lot of superior advantages, such as good power density, long cycle life, short charge/discharge time, and of course no negative effect to the environment. The most significant way to design/construct a supercapacitor is to find a kind of electrode material with outstanding performance, Generally It is anode [10]. Due to its 2D sheet like structure MoS2 attracted a lot of researchers to use it as anode material in supercapacitors. Sheet like structure of MoS2 provides a large surface area for double-layer charge storage. MoS2 will always be considered a better supercapacitor material as it has higher intrinsic fast ionic conductivity in comparison of metal oxides and graphite. So far, many research groups have given their best effort to exploit the electrochemical as well as mechanical performance of MoS2.

Literature review

Ab initio method based study In 2012, Siqi Yang et al studied Zigzag MoS2 nanoribbon structure for cathode material of rechargeable Mg batteries using first principle based on density functional theory (DFT) [7]. Their study has been carried out on this material concentrated on various key issues like magnesium adsorption sites, theoretical capacity, and diffusion kinetics. The activation barrier for this material is only 0.48 eV, which is much reduced from the 2.61 eV of the bulk interlayer-migration.

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In March 2018, Yujun ji et al worked on the restriction of the performance of MoS2 based supercapacitors. They restricted the performance of MoS2 by using limited ionic intercalation in the molecular layer of MoS2. [11] To find the solution of this situation they synthesized the high-density edge oriented MoS2 Nano sheets with an expanded interlayer spacing of 9.4 angstrom supported on reduced graphene oxide. The specific capacitance reported by them up to 346.5 F g–1 at a scan rate of 1 mV s–1, which is significantly higher than most reported values in the past in supercapacitors using different type of MoS2/graphene composites.

In April 2018, Mohit Saraf et al have worked on supercapacitor properties of a molybdenum disulfide–reduced graphene oxide (rGO) heterostructure-based binder-free electrode. This rGO delivered a high specific capacitance (387.6 F g–1 at 1.2 A g–1) as well as impressive cycling stability [17]. Additionally, the future role of rGO in the composites of MoS2 for supercapacitor designing are also discussed in brief.

In May 2018, D. N. Sangeetha et al have worked on active-defective activated carbon, MoS2 composites for supercapacitors [9]. They worked on temperature tuned synthesis of dual phase MoS2. They prepared high specific surface area activated carbon using Diospyros Melanoxylon leaves (common name Tendu leaves). Displays Enhanced specific capacitance is used to fabricate the symmetric and hybrid activated carbon/ MoS2 supercapacitors.

In June 2018, Chandu Nagaraju et al worked on Hydrothermal synthesis of MoS2 to enhance its specific capacitance [15]. The results investigated by them for the electrochemical properties of MoS2, specific capacitance (Cs) of 1531.2 F g−1 at 5 mA cm−2 with good cycling stability (up to 81.6% retention over 3000 cycles). They worked with WS2 also. The WS2 electrode also delivers an enhanced specific capacitance of 1439.5 F g−1 at 5 mA cm−2.

In May 2018, K. Chanda et al worked on Hierarchical heterostructure of MoS2 Flake Anchored on TiO2 Sphere for Supercapacitor Applications [16]. They synthesized TiO2 spheres using titanium iso-prop oxide assisted hydrothermal route. After that secondary growth of MoS2 was accomplished. This synthesized hybrid material shown significantly improved electrochemical behavior than pristine TiO2 sphere. The specific capacitance for the hybrid is changed to 152.22 F/g at current density of 0.1 A/g which is a significant improvement. They said that enhance in properties is due to high surface area of the hybrid sample.

Molecular dynamics based study

In June 2018, Zheng Bo et al worked on the design of supercapacitors using molecular dynamic simulations. They worked on EDLCs (Electric double layer capacitors) for enhancing its efficiency in the term of storing and charging cycles as well. Molecular dynamic investigation of 2D 1D and 0D materials for finding the change in

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specific capacitance [6]. They conclude that molecular dynamic study can lead to the optimization of electron density inside carbon electrode at atomic level.

In July 2015, Mark A. Bissett. et al studied the characterization of MoS2 composites for enhancing the performance of coin cell supercapacitor [8]. They conclude that composite membrane made from solution exfoliated dispersion of semiconducting MoS2 can create synergistic effect that lead to the construction of high-performance supercapacitors. MoS2 has high specific capacitance with very less mass loading. They also observed that electro activation due to ion intercalation leads to a significant increment in specific capacitance of MoS2

In August 2016, Sujin P. Ghose et al worked for enhancing supercapacitor performance of 3D architecture using rGO-MoS2 2D sheets. They fabricated a robust 3D architecture by the use of 2D Nano-sheets of GO and MoS2 as the building blocks [3]. This architecture has very high specific capacitance. Integration of graphene into the structure provides significantly large surface areas for the loading of MoS2 petals.

In 2017, Sungwook Hong et al worked on computational synthesis of MoS2 layers using molecular dynamics simulation. They investigated the synthesis of MoS2 layers from deposited MoO3 by the use of reactive force field/reactive molecular dynamics simulations with re-optimized force field parameters for Mo/O/S [4]. Their approach is very modern in this field; it can open a new direction to explore different processes for synthesis of MoS2 monolayers.

Conclusions and future scopes

The exceptional and outstanding performance of the MoS2 electrode indicates its potential application in next-generation high-performance supercapacitors. Reviews show that the effective specific capacitance can be enhanced of 2D Nano materials for the application of energy storage either by synthesis and doping of new materials or by creating defects in the crystal structure of the material.

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List of Figures

Figure no.1*Mg Absorption in MoS2 (with permission from ACS Publications for use in this paper)*

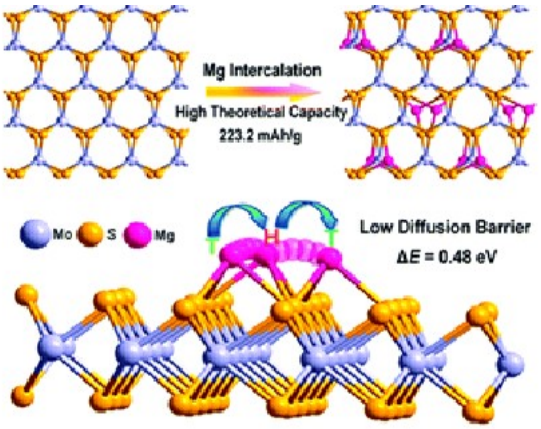

Figure 2*Design of Supercapacitor Electrodes Using Molecular Dynamics (with permission from Springer Publications for use in this paper)*