Ab-Initio Simulations Accelerate the Development of High-Performance Lithium-Sulfur Batteries

Published as part of the Virtual Special Issue "Beihang University at 70"

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Abstract

Lithium-sulfur batteries (LSBs) are promising candidates for next-generation cost-effective and high-energy-density rechargeable batteries. However, cathodes, anodes, and electrolytes of LSBs all face multiple technological challenges. Nowadays, theoretical models play an increasingly important role in LSBs in probing highly catalytic cathodes, dendrite-free anodes, and stable electrolytes. In this perspective, first, the LSBs theoretical research projects our group participated in are reviewed, focusing on highlighting the interpretation and guidance of ab-initio simulations on experiments. Next, the prospect of combining automated workflow managers, machine learning techniques with ab-initio simulations is presented, hoping to introduce a new paradigm for LSBs research and development.

Key words: Ab-initio simulations; Automated workflow managers; Lithium anodes; Sulfur cathodes

1 Introduction

For decades, lithium-ion batteries (LIBs) have played an important role from mobile electronic devices to electric vehicles. Given the contribution of LIBs to society, the 2019 Nobel Prize in Chemistry was awarded to three scientists working on LIBs. However, the advent of the ever-increasing demand for power sources eagerly urges us to search for new energy storage systems beyond present LIBs.[1] Featuring high specific capacity, low cost, and environmental benignity of sulfur, lithium-sulfur batteries (LSBs) have been regarded as a promising candidate for the next generation of high-performance energy conversion and storage techniques with carbon-neutral capability.[2] Nevertheless, technological challenges arising from the sulfur (S) cathode (low conductivity, shuttle effect and sluggish conversion reactions), the lithium (Li) anode (dendrite growth) and the electrolyte (lithium polysulfide dissolution and gas evolution) prevented the practical application of LSBs (Fig. 1).[3,4] Nowadays, theoretical models play an increasingly important role in Li-S systems in probing highly catalytic cathodes and dendrite-free anodes as well as exploring the conversion reaction mechanism. In this perspective, we will review the LSBs theoretical research projects our group participated in, focusing on highlighting the interpretation and guidance of ab-initio simulations on experiments. Then, we will present the prospect of combining automated workflow managers, machine learning techniques with ab-initio simulations in the development of LSBs.

2 The S Cathodes

2.1 Challenges Facing S Cathodes

The major challenges of the S cathode include low electronic/ionic conductivity of S_8 and Li_2S_2/Li_2S, the shuttle effect of lithium polysulfides (LiPSs), the sluggish conversion reactions and the large volume change during charging and discharging.[3,4] To overcome these challenges, carbon-based materials were firstly used as S host materials.[5,6] Carbon materials possess excellent electronic conductivity and various forms such as carbon black, graphite, carbon nanomaterials and porous carbon.[5] Combining different forms of carbon materials into carbon-based composites as S hosts can solve the problems of low conductivity and large volume change.[6] Since carbon-based materials have an adsorption effect on LiPSs, they can also inhibit the diffusion of LiPSs in the electrolyte to a certain degree.[5] However, the interaction between non-polar carbon-based materials and polar LiPSs is weak. Thus, the surfaces of carbon-based materials were modified to introduce polar sites, and polar materials such as metal oxides and sulfides were adopted to achieve stronger chemical anchoring on LiPSs.[3,5] For example, Hou et al.[7] theoretically investigated heteroatom-doped carbon materials and found a significant enhancement to the anchoring effect of N or O doped carbon compared with undoped carbon. Chen et al.[8] systematically studied first-row transition-metal monosulfides as polar S hosts. It is found that, the adsorption energy between VS and Li_2S molecule is −4.89 eV, which is much greater than that between graphene and Li_2S. Never-
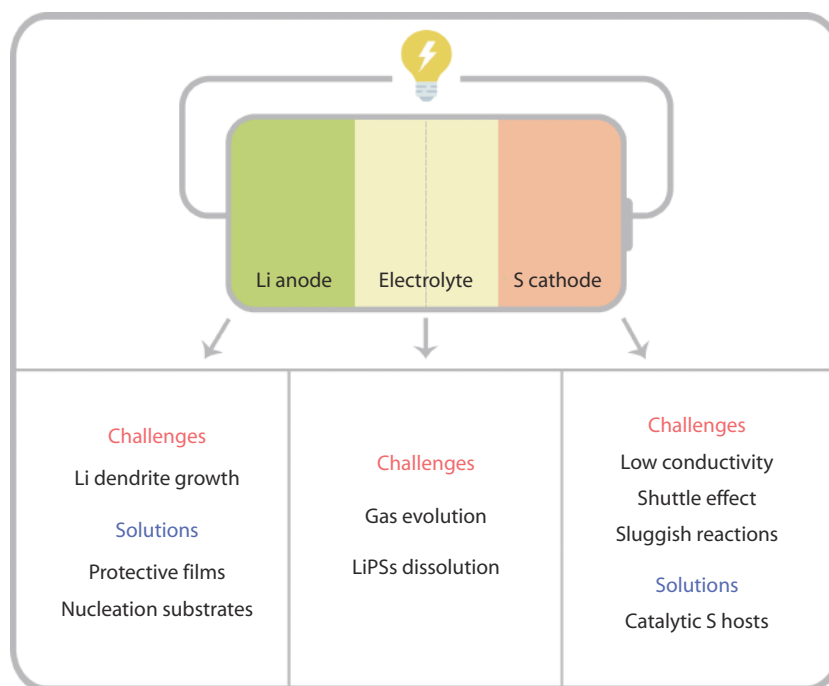
Fig. 1 Challenges of Li-S batteries and their possible solutions.

theless, the adsorption sites will be saturated if LiPSs are only passively adsorbed. It is more important to actively catalyze the conversion of LiPSs at the same time of adsorption, so the concept of catalysis was introduced into the design strategy of S host materials.[4] For example, Lian et al.[9] studied the supported single-atom catalyst (SAC) on nitrogen-doped graphene using the crystal graph convolutional neural network (CGCNN). They concluded that supported SACs such as Ti, V, Zr, Mo, and Os are promising candidates for cathode catalysts of Li-S batteries.

2.2 Metal Sulfides as S Hosts

According to the design strategy mentioned above, we studied various S host materials, among which metal sulfides (M_xS_y) were the most deeply studied.[10–12] We firstly investigated the anchoring effect of M_xS_y on LiPSs and theoretically explained why LiPSs can be effectively anchored by some M_xS_y.[10,11] Ab-initio simulations showed that the binding energy between two-dimensional (2D) layered TiS_2 and Li_2S molecule is 2.99 eV (Fig. 2a),[10] which is 10 times higher than that between a single layer of graphene and Li_2S molecule (0.29 eV).[14] This suggests a strong anchoring effect of TiS_2 on LiPSs because of the similar chemical bonding nature between LiPSs and Li_2S molecule.[15,16] Using $Li_2S@TiS_2$ as cathode material, the specific capacity reached 503 mAh g^{-1} Li_2S (~722 mAh g^{-1} S) at a high rate condition of 4C, which can be attributed to the strong chemical anchoring effect on LiPSs and the greatly enhanced conductivity of $Li_2S@TiS_2$. In addition to 2D layered TiS_2, 2D layered ZrS_2 and VS_2 also achieved good performance as S host materials.[10] To explain the anchoring effect of these M_xS_y on LiPSs, we calculated binding energies between various kinds of 2D materials (such as metal oxides, sulfides, and chlorides) and LiPSs (Fig. 2b).[11] We found that the anchoring of LiPSs is accompanied by the weakening of Li-S bonds of LiPSs. Weak anchoring materials, such as $ZrCl_2$, cannot confine LiPSs on their surfaces, while strong anchor-

ing materials, such as V_2O_5, with binding energies greater than ~2.0 eV, will lead to the decomposition of LiPSs. Only moderate anchoring materials, such as TiS_2, ZrS_2 and VS_2, can both confine LiPSs on their surfaces and preserve the structures of LiPSs, thus achieving a better anchoring effect.

We also studied the catalytic effect of M_xS_y on Li_2S during charging.[12] Through ab-initio simulations, we simulated the band structures of a series of M_xS_y, and calculated the binding energies between Li_2S_6 molecule and these M_xS_y, the diffusion energy barriers of Li ion on the surfaces of these M_xS_y and the decomposition energy barriers of Li_2S molecule on the surfaces of these M_xS_y (Fig. 2c). The calculated results indicated that, the intrinsic conductivity, the strong anchoring effect on LiPSs and the assistance to Li ion diffusion of M_xS_y are important to reduce the decomposition energy barrier of Li_2S and improve the battery performance. For all the metrics mentioned above, VS_2 possesses the best performance among all M_xS_y, which was further confirmed by experiments.[12] Besides M_xS_y, we also studied many other S host materials such as amphiphilic polymer modified hollow carbon nanofibers,[14] conductive polymers,[17,18] MoS_2,[19] MoS_3,[20] MoO_3[21] and single-atom metal@nitrogen-doped graphene (SAM@NG),[22] all of which improved the battery performance.

3 The Li Anodes

3.1 Challenges Facing Li Anodes

The major challenge of the Li anode is the growth of Li dendrites.[3] The uneven deposition of Li ions on the surface of Li metal will lead to the growth of Li dendrites, which may penetrate the separator and contact with the cathode, releasing a lot of heat in a short period of time and resulting in safety hazards such as burning or even explosion. To solve this problem, the concepts of protective films and nucleation
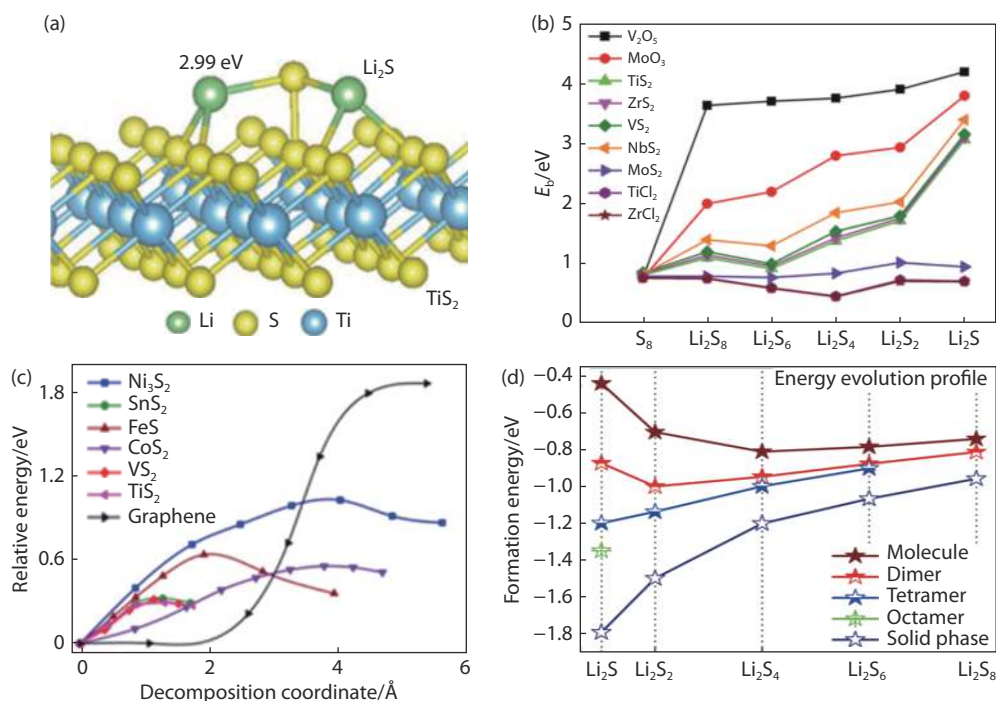
Fig. 2 Ab-initio simulations improving the performance and revealing the mechanisms of S cathodes. (a) The most stable configuration of a Li_2S molecule adsorbed on a single layer of TiS_2 with an adsorption energy of 2.99 eV.[10] Copyright 2014, Macmillan Publishers Limited. (b) Binding energies between Li_2S_n (n = 1, 2, 4, 6, 8) and various 2D anchoring materials.[11] Copyright 2015, American Chemical Society. (c) Decomposition energy barriers of Li_2S molecule on the surfaces of a series of M_xS_y.[12] Copyright 2017, National Academy of Sciences. (d) Formation energy evolution profile of Li_2S_n (n = 1, 2, 4, 6, 8) from small molecules to large clusters and solid phases.[13] Copyright 2019, American Chemical Society.

substrates were proposed. For protective films, firstly they are highly ionically-conducting, thus offering diffusion pathways for Li plating/stripping. Secondly, they have excellent mechanical performance, thus suppressing the growth of Li dendrites. For nucleation substrates, due to their lithiophilic surfaces, Li ions tend to deposit uniformly, thus inhibit the Li dendrites growth.

3.2 Protective Films

Using ab-initio simulations, we systematically investigated the performance of eight types of 2D materials as protective films.[25] We found that introducing defects, increasing the size of hollow rings of the structure and the metal proximity effect on protective film can improve the conductivity of Li ions but decrease the mechanical performance of protective films at the same time. Thus, to achieve better performance of the protective film, it is necessary to make a rational compromise between ionic conductivity and mechanical strength. According to the design strategy mentioned above, we investigated the possibility of bi-layer artificial solid electrolyte interface (SEI) consisting of covalent graphitic layer and inorganic layer as a protective film.[26] Since the graphitic layer has good mechanical properties, it can be placed on the Li metal side to suppress the growth of Li dendrites, and the inorganic layer can be placed on the electrolyte side to protect the graphitic layer from corrosion by organic components in the electrolyte. Simulations indicate that LiF < 111 > based bilayer artificial SEI has good stability, ionic conductivity and mechanical strength, representing a promising candidate for Li anode protective films.

3.3 Nucleation Substrates

For nucleation substrates, we firstly investigated the nitrogen-doped graphene with atomically dispersed single-atom Ni (SANi-NG) (Fig. 3a).[23] Simulations indicated that the single-atom Ni on NG can not only enhance the lithiophilicity of the substrate surface by adsorbing Li with adsorption energy (1.92 eV) larger than the Li cohesive energy (1.63 eV) and a moderate adsorption energy gradient (Fig. 3b), but also enhance the structural stability of the entire nucleation substrate during Li plating/stripping. Secondly, sulfur-doped graphene (SG) was also studied by ab-initio simulations.[24] We found that the S atoms doped on graphene sacrifice the Li adsorption ability of its nearest regions, but uniformly enhance the Li adsorption ability of its distant regions, thus increasing the lithiophilicity of the entire surface with a moderate gradient by a small amount of S atoms doping (~2.0 at%) (Fig. 3c and 3d). Experiments confirmed that compared with pristine graphene, using SANi-NG or SG as nucleation substrate can effectively reduce the number of Li dendrites on their surfaces after Li plating/stripping by scanning electron microscopy.[23,24] The dendrite free Li nucleation and plating process is illustrated in Fig. 3e.

Other researchers also achieved fruitful theoretical insights into nucleation substrates. For example, Chen et al.[27] systematically studied the lithiophilicity chemistry of heteroatom-doped carbon materials. O-doped and O/B-co-doped carbons were recommended for their highest lithiophilicity among single-doped and co-doped carbons, respectively. Ma et al.[28] studied the defect chemistry of carbon frameworks and the Stone-Wales defect was found to be helpful in deliv-
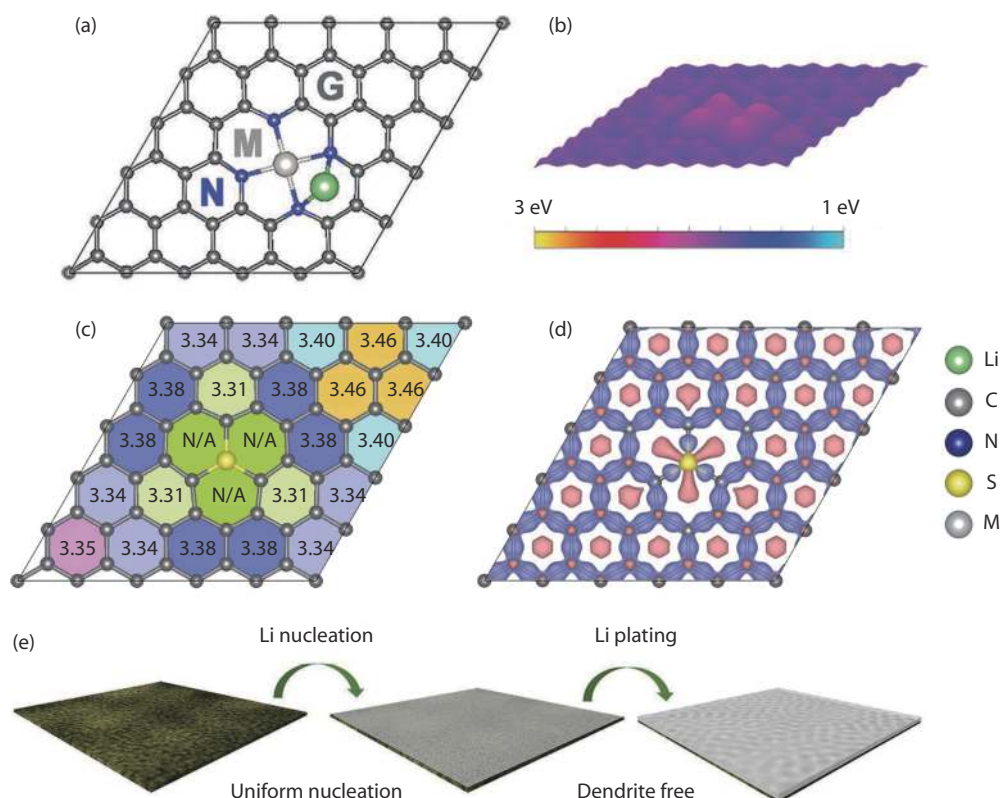
Fig. 3 Ab-initio simulations assisted development of dendrite free Li anodes. (a) The configuration of Li adsorbed on SA metal-NG.[23] Copyright 2019, WILEY-VCH. (b) Distribution map of binding energies of Li on different adsorption sites of SA metal-NG.[23] Copyright 2019, WILEY-VCH. (c) Distribution map of binding energies of Li on different adsorption sites of SG.[24] Copyright 2019, WILEY-VCH. (d) Charge density difference of SG. Charge accumulation and loss are represented by violet and pink, respectively.[24] Copyright 2019, WILEY-VCH. (e) A dendrite free Li nucleation and plating process.[23] Copyright 2019, WILEY-VCH .

ering a uniform Li deposition. Jiao et al.[29] performed molecular dynamics (MD) to study the self-healing mechanisms in Li metal using a machine learning based Li potential and both the surface self-healing and the bulk self-healing mechanisms were proposed.

4 The Electrolytes

In addition to the electrode systems, the development of electrolyte in Li-S batteries also faces multiple challenges. On the one hand, as mentioned in the S cathode section, LiPSs are able to dissolve in the electrolyte, leading to the shuttle effect and the loss of active materials. On the other hand, due to the low negative electrochemical potential of the Li metal anode, the electrolyte can be reduced to combustible gases and caused the safety hazard.

In order to suppress the dissolution of LiPSs in the electrolyte, we should first have a more accurate understanding of the condensed form of LiPSs in the electrolyte. We revealed a more realistic LiPSs conversion process through ab-initio simulations.[13] People conventionally regard LiPSs as molecules. However, in well encapsulated cathodes, LiPSs may tend to exist as aggregated phases. Using the structure prediction technique, we identified structures of LiPSs from small molecules to large clusters and to solid phases. We calculated the phase diagram and the formation energy evolution profile (Fig. 2d), which demonstrated a strong cohesive tendency of

Li_2S and Li_2S_2, and a moderate cohesive tendency of Li_2S_4 and Li_2S_6. Using this model, we investigated the dissolution and the conversion of LiPSs, and successfully explained the formation of the voltage dip and why there are two voltage plateaus during discharging and one flat voltage plateau during charging, confirming the reasonability of our LiPSs conversion model.

Other researchers also obtained insightful results. Rajput et al.[30] and Kamphaus et al.[31] studied the solvation structures and dynamics of the polysulfide species in different composition of electrolytes using MD method with classical potential and proposed valuable strategies to reduce the solubility of LiPSs. Through multiscale ab-initio simulations, Chen et al.[32] investigated the gas evolution mechanisms in Li-S battery using 1,3-dioxolane (DOL)/1,2-dimethoxyethane (DME) as the electrolyte and found that the adsorption of Li can make the decomposition energy barriers of DOL and DME lower, which increases the gas generation.

5 Future Perspectives

Previous studies have offered many valuable design strategies for Li-S battery materials, such as the design strategies for catalytic S hosts, Li anode protective films and Li nucleation substrates mentioned above. However, the application of these design strategies is insufficient. Due to the limitation of time and energy, researchers usually screen materi-

als that meet the design strategy among several to dozens of common materials, but overlook the huge database of battery materials. Recently developed automated workflow managers added new features of high-throughput and automation to ab-initio simulations, making it ideal for screening the optimal Li-S battery materials out of the entire battery materials database.[33–36] Automated workflow managers can handle tedious and repetitive work, so that researchers can free themselves from input file preparation, job submission and result analysis and fully focus on the design of the screening workflow of Li-S battery materials. If combined with structure prediction techniques,[37,38] it can also explore an unprecedented material searching space full of opportunities.

Machine learning plays an important role in the research and development of Li-S batteries from the microscale to the macroscale.[39] For example, at the microscale, machine learning can be used for the construction of functionals in density functional theory (DFT) and the construction of potentials in MD. Such methods can greatly improve the calculation speed while maintaining the simulation accuracy, which is beneficial to the large-scale and long-term research; at the macroscale, machine learning can be used to predict the battery lifespan and optimize the fast-charging protocol, which is crucial for the practical applications of Li-S batteries. Thus, even materials with poor properties can contribute to the fitting of the structure-property relationship. Ab-initio simulations, especially combined with workflow managers and machine learning techniques, will be important tools for accelerating the research and development of Li-S batteries in the future.

Acknowledgements

Conflicts of interest

The authors declare no conflict of interest.

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