

锂硫电池用铁基化合物催化剂的研究现状

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收稿日期: 2024年1月17日; 录用日期: 2024年2月21日; 发布日期: 2024年2月29日

摘要

锂硫电池因具有突出理论比容量和能量密度而被认为是有望替代锂电池的新一代储能系统的强有力竞争者。但它所存在的穿梭效应等问题导致了电池容量的快速下降和差的循环稳定性, 阻碍了锂硫电池商业化的进程。过渡金属化合物普遍具有优异的催化性能以及独特的电子结构, 其中的铁基化合物因其低成本、良好的导电性以及强的催化活性获得了广泛的关注。本文重点综述了锂硫电池用铁基化合物催化剂的最新进展, 并展望了其未来的发展趋势。

关键词

锂硫电池, 铁基化合物, 催化剂

Research Status of Iron-Based Compounds as Catalysis for Lithium-Sulfur Batteries

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Received: Jan. 17th, 2024; accepted: Feb. 21st, 2024; published: Feb. 29th, 2024

Abstract

Lithium-sulfur battery was regarded as a strong competitor to the next generation of energy storage systems that are expected to replace lithium-ion batteries due to their outstanding theoretical specific capacity and energy density. However, the shuttle effect and other issues resulted in a rapid decrease in battery capacity and poor cycling stability, hindering the commercialization process of lithium-sulfur batteries. Transition metal compounds generally exhibit excellent catalytic performance and unique electronic structures, among which iron-based compounds have re-

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ceived widespread attention due to their low cost, excellent conductivity, and strong catalytic activity. This article focuses on the latest progresses of iron-based compounds used as catalysts for lithium-sulfur battery, and looks forward to their future development trends.

Keywords

Lithium-Sulfur Batteries, Iron-Based Compounds, Catalysis

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1. 引言

随着科技的进步和社会的发展,煤炭、石油等化石能源正在枯竭,寻找一种能够替代的新能源体系迫在眉睫[1]。各类可再生能源的不稳定性以及现有的以锂电池为主的储能系统低的理论容量,都越来越难以满足发展的需求。超级电容器[2]、钠离子电池[3]、空气电池[4]以及锂硫电池[5]等新型的储能系统得以被广泛的研究开发。

硫正极材料具有的如低成本、丰富的储量等固有特性使得锂硫电池系统成为了下一代储能系统的强有力的竞争者。但体积变化、穿梭效应、锂枝晶的生成以及不稳定性等问题阻碍了锂硫电池的进一步发展[6] [7] [8],需要研究者提出科学有效的解决方案。研发正极载体材料[9]、改性隔膜和调整电解液配方等[10]方案均已被提出并进行了大量的研究。其中最有效简单的方案是开发合适的极性催化剂用以促进多硫化物(LiPSs)的化学吸附和催化转化以抑制穿梭效应,图1展示了穿梭效应的机理。

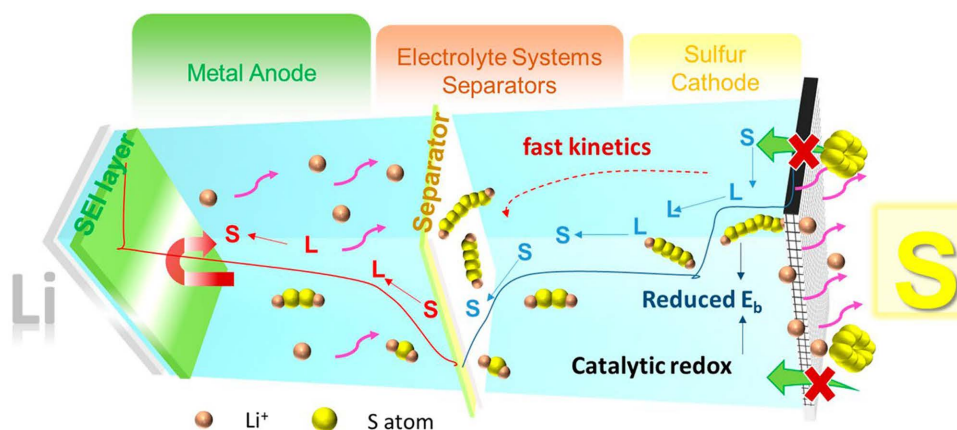


Figure 1. Schematic illustrations of shuttle effect [11]

图1. 穿梭效应示意图[11]

铁基化合物作为最为常见的过渡金属材料之一,在锂离子电池和各类能源存储领域具有广泛的运用。其中,氧化铁[12]、碳化铁[13]、磷化铁[14]、硫化铁[15]等铁基化合物具有良好的极性和催化活性,可以通过极性-极性相互作用化学地捕获可溶性LiPSs,并且促进其快速转化。然而,不同种类的铁基化合物在锂硫电池中起到的作用不尽相同,为了更好的筛选铁基催化剂材料,我们总结并介绍了近几年各类铁基化合物用于锂硫电池的研究现状(如图2),并分析了其在锂硫电池应用中面临的困难挑战和前景。

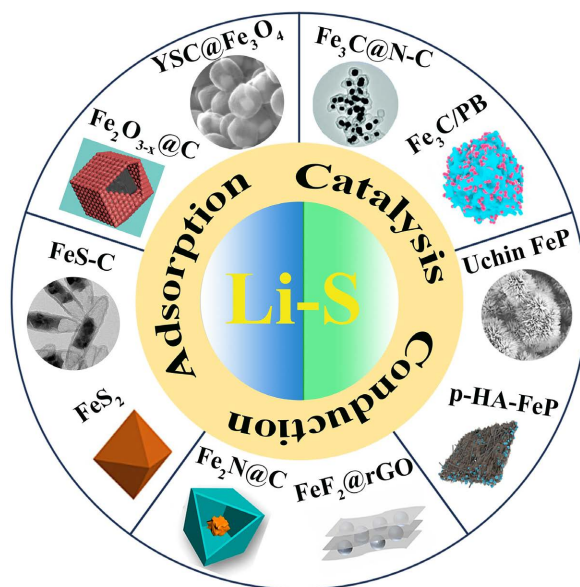


Figure 2. Display diagrams of various iron-based compounds used in the research of lithium-sulfur batteries
图 2. 目前用于锂硫电池研究的各类铁基化合物的展示图

2. 锂硫电池中铁基化合物的研究进展

2.1. 氧化铁

氧化铁(包括 FeO , Fe_2O_3 , Fe_3O_4)因为成本低、容易获得、表面官能团强等,能够有效的捕获可溶多硫化锂抑制穿梭效应。早在 2014 年, Han 等[16]利用普鲁士蓝作为原材料制备得到了大小均匀的多孔 Fe_2O_3 微立方体,使用其作为正极载体的锂硫电池首次观察到较高比容量和稳定的电化学循环,这意味着 LiPSs 的穿梭得到了明显的缓解。然而,氧化铁材料本征导电性低,且单一氧化铁材料尺寸难以控制,导致了活性位点的缺乏和稳定性不足。通过水热等原位合成方法有效强化了材料的空间容量并调控了材料尺寸(如图 3(a)) [17] [18],复合材料表现出增强的 LiPSs 吸附和快速的氧化还原反应动力学,有效地抑制了 LiPSs 的穿梭和提高了硫的利用率。核壳结构[12] [19] [20]的设计(如图 3(b))在空间上结合了氧化铁磁芯对 LiPSs 的强化学相互作用与导电碳壳提供的高效电子传输通道,保障了锂硫电池出色的速率性能,高容量和长循环寿命。原位测试(如图 3(c))为电池的长期循环稳定性和高的库伦效率提供了合理的解释 [12]。DFT 计算(图 3(d))结果从理论上揭示了 Fe_3O_4 对 Li_2S_n 的强力极性-极性相互作用[21],论证了实验结论的理论正确性。Li 等[22]采用冷冻干燥法制备精细分散在氮掺杂多孔碳上的纳米级的 Fe_3O_4 (nano- $\text{Fe}_3\text{O}_4/\text{PNC}$),如图 3(e)所示,纳米级的 Fe_3O_4 可以有效捕获 LiPSs,高分散性为 LiPSs 的催化转化提供了大量的反应位点。氧空位工程[19] [23]能够调节电子结构(如图 3(f)),为改善电化学性能暴露更多的活性位点,在不牺牲活性位点的前提下提供了出色的倍率性能和稳定性。同一材料的不同晶面所具有的化学性质不尽相同, Li 等[24]通过实验探究了调控 $\alpha\text{-Fe}_2\text{O}_3$ 不同晶面生长的方法,并利用 DFT 计算对比了 LiPSs 在 $\alpha\text{-Fe}_2\text{O}_3$ 的(110)和(104)晶面上吸附能的差异(如图 3(g))。这为探索不同晶面金属氧化物对 LiPSs 的吸附能力提供了新的思路,为商业化开辟了可能性。综上所述,氧化铁本身具有极性和中等的催化活性,可以实现 LiPSs 的吸附-催化转化。而氧化铁材料与石墨烯、多孔碳等多孔材料的复合,可以改善电池电化学性能。此外,氧化铁的结构纳米化有助于提高催化活性并且为 LiPSs 的氧化还原反应提供大量的反应位点,有效地抑制 LiPSs 的穿梭效应,极大地改善了循环稳定性。

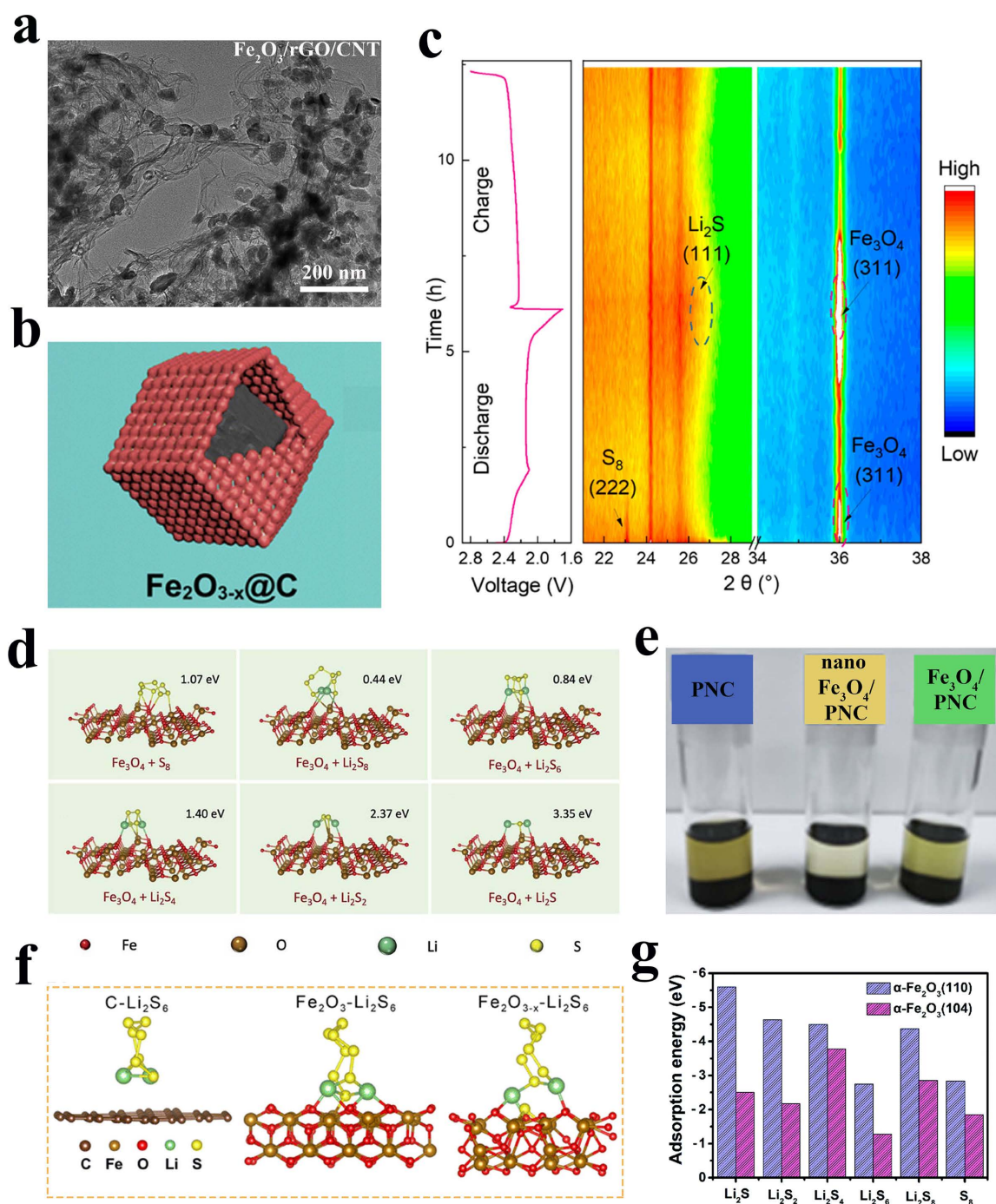


Figure 3. (a) TEM image of $\text{Fe}_2\text{O}_3/\text{rGO}/\text{CNT}$ [17]. (b) Structure diagram of $\text{Fe}_2\text{O}_{3-x}@\text{C}$ [19]. (c) In situ XRD contour plots of S/YS-27 $\text{Fe}_3\text{O}_4@\text{C}$ electrode in the first discharge/charge process within the voltage window of 1.7~2.8 V [12]. (d) DFT-calculated molecular structures and adsorption energies of Li_2S_n and S_8 on Fe_3O_4 [21]. (e) Optical photographs of Li_2S_6 solution treated with PNC, nano- $\text{Fe}_3\text{O}_4/\text{PNC}$, and $\text{Fe}_3\text{O}_4/\text{PNC}$ for 30 min [22]. (f) Optimized configurations of Li_2S_6 molecule on different surfaces [19]. (g) Adsorption energies of the S_8 cluster and Li_2S_x ($x = 1, 2, 4, 6, \text{ and } 8$) on the (104) and (110) facets of $\alpha\text{-Fe}_2\text{O}_3$ [24]

图 3. (a) $\text{Fe}_2\text{O}_3/\text{rGO}/\text{CNT}$ 的 TEM 图像[17]。 (b) $\text{Fe}_2\text{O}_{3-x}@\text{C}$ 的结构示意图[19]。 (c) 使用 S/YS-27 $\text{Fe}_3\text{O}_4@\text{C}$ 作为正极的锂硫电池在 1.7~2.8 V 电压范围内首圈充放电的原位 XRD 等高线图[12]。 (d) Li_2S_n 以及 S_8 在 Fe_3O_4 表面吸附的 DFT 计算模型和吸附能[21]。 (e) PNC, nano- $\text{Fe}_3\text{O}_4/\text{PNC}$ 以及 $\text{Fe}_3\text{O}_4/\text{PNC}$ 吸附 Li_2S_6 溶液 30 分钟后的可视化图[22]。 (f) Li_2S_6 在不同表面上的优化构型[19]。 (g) S_8 团簇和 Li_2S_x ($x = 1, 2, 4, 6$ 和 8) 在 $\alpha\text{-Fe}_2\text{O}_3$ 的(104)和(110)晶面的吸附能[24]

2.2. 碳化铁

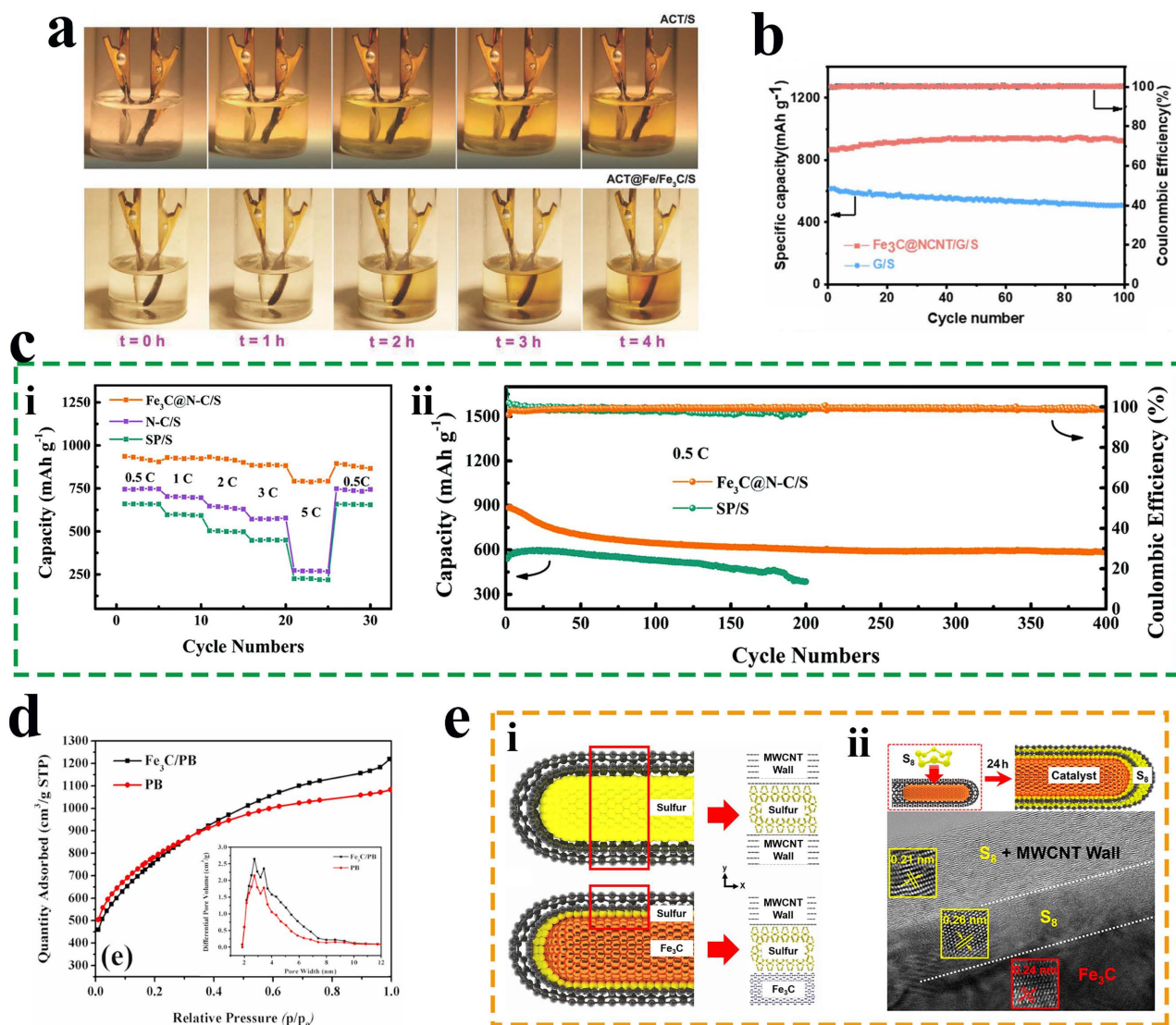


Figure 4. (a) Digital images of the ACT/S composite and ACT@Fe/Fe₃C/S composite electrodes during the first discharge cycle in the liquid cell at the current density of 0.1 C [25]. (b) Long-term cycling performance of Fe₃C@NCNT/G/S cathode at 1 C [13]. (c) i): The rate capability of Fe₃C@N-C/S, N-C/S and SP/S at increasing current rates from 0.1 C to 5 C; ii): cycling performance at 0.5 C [26]. (d) N₂ adsorption/desorption isotherm and pore size distributions (insert) of Fe₃C/PB and PB [30]. (e) i): MD atomic structures of the S/MWCNT and S/Fe₃C/MWCNT; ii): Sulfur infiltration process and HRTEM image of the nanotube wall, sulfur, and Fe₃C particle [31].

图 4. (a) ACT/S 复合物和 ACT@Fe/Fe₃C/S 复合电极在液体电池中 0.1 C 电流密度下首次放电循环下的可视化图片[25]。(b) Fe₃C@NCNT/G/S 正极在 1 C 下的长循环[13]。(c) i): Fe₃C@N-C/S, N-C/S 和 SP/S 电极在 0.1~5 C 范围内的倍率性能; ii): 在 0.5 C 的长循环性能[26]。(d) Fe₃C/PB 和 PB 的氮气吸附/脱附曲线和孔径大小分布曲线(内置) [30]。(e) i): S/MWCNT 和 S/Fe₃C/MWCNT 的 MD 原子结构; ii): 硫的渗透过程和 MWCNT、S₈ 以及 Fe₃C 颗粒的 HRTEM 图像[31]

碳化铁(Fe₃C)因其固有的磁性和优异的催化活性等特点,在锂硫电池上表现出特殊的 LiPSs 捕获方式和显著的催化能力。Gao 等[25]提出了 Fe₃C 存在于电池正极时,通过磁性形成内部磁场,能够以洛伦兹力改变 LiPSs 的溶解路径,从而促进 LiPSs 的捕捉,并将这种独特的机制被称为“屏蔽效应”。从图 4(a) 可以看到, ACT@Fe/Fe₃C/S 电极利用本征电场有效的将 LiPSs 限制在正极一侧,自发捕获 LiPSs 以提高

硫的利用率。此外, Fe_3C 表现出优异的 LiPSs 催化活性, 可以促进 LiPSs 快速转化。这种强力锚定作用和高的催化转化能力, 有效抑制了 LiPSs 的穿梭。电磁性材料对 LiPSs 独特的捕获机制有希望最大限度的利用 LiPSs 并减轻穿梭效应, 具有提高 LiPSs 利用率以及降低穿梭效应的可行性。将 Fe_3C 负载在具有杂原子氮掺杂的碳材料上已经是一种提高循环稳定性的极为可行的方案[13] [26] [27] [28], 氮掺杂使碳材料获得了一定的导电性, 结合 Fe_3C 对 LiPSs 转化的催化效果得到了更好的电池性能(如图 4(b)), 大量的氮掺杂碳材料通过富含氮元素的前驱体如多巴胺和三聚氰胺等制备得到[29]。不同形貌碳材料的加入以及杂原子的掺杂在一定程度上有效提高了材料的导电性, 为离子扩散和电子转移提供了更丰富的活性位点。Zhang 等[26]模仿青蛙卵结构设计了空心 $\text{Fe}_3\text{C}@N\text{-C}$, 大孔结构有效提高了硫的容纳率并能够缓解硫物种的体积变化, 良好的导电性有利于离子传输, 有效降低电池内阻并加速硫物种的转化。核壳结构材料实现了同位点进行体积缓解和催化转化的结合, 提供了卓越的倍率性能以及出色的循环稳定性(如图 4(c))。

此外, 使用生物质碳材料作为 Fe_3C 的基底材料, 其极高的比表面积和孔隙结构有利于缓解充放电过程中的体积变化, 简单安全制备过程也便于大规模工业化生产。Lei 等[30]提出了一种利用苏铁叶同步碳化和 Fe_3C 掺杂制备多功能复合材料 $\text{Fe}_3\text{C}/\text{PB}$ 的一步法策略, Fe_3C 纳米颗粒得以均匀分布在生物炭表面, 与硫结合后产生的 Fe-S 键证实了其对穿梭效应的缓解能力。高达 $2723 \text{ cm}^2 \cdot \text{g}^{-1}$ 的比表面积(如图 4(d))提供了大量的活性位点, 极高的孔隙体积为缓解体积膨胀做出了巨大的贡献。Cheng 等[31]以棉花为原料大规模的制备了多壁碳纳米管封装 $\text{Fe}/\text{Fe}_3\text{C}$ ($\text{Fe}/\text{Fe}_3\text{C}\text{-MWCNT}$), 利用生物纤维素热解产生的气体进一步影响材料的孔结构并帮助 $\text{Fe}/\text{Fe}_3\text{C}$ 在空隙中生成, 碳化生成的无定形碳能够进一步石墨化生长成碳纳米管并对原位生成的 $\text{Fe}/\text{Fe}_3\text{C}$ 进行封装。如图 4(e)所示, 仿真和计算结果都证明了 Fe_3C 纳米颗粒对碳纳米管在充放电过程中形变的缓解, 这抑制了 LiPSs 的溶解, 保障了对硫物种的收纳帮助提供优越的循环性能。总之, Fe_3C 独特的磁性、电子结构和催化能力有利于它们在锂硫电池中的应用。

2.3. 磷化铁

作为一种高效的电催化剂, 磷化铁(FeP , Fe_2P 和 Fe_3P)具有良好的导电性、热稳定性以及化学稳定性等, 同时, 磷的独特的电子轨道分配提高了磷化物催化剂的活性[32] [33], 促进了磷化铁在催化和储能系统中的应用。Huang 等[34]报道了一种掺入 3D 多孔石墨烯 - 碳纳米管支架上的磷化铁纳米晶体 ($\text{FeP}/\text{rGO}/\text{CNTs}$), 用于稳定和高倍率的锂硫电池。如图 5(a), DFT 理论计算表明 FeP 对 LiPSs 具有强力的化学吸附, 从而抑制 LiPSs 穿梭效应。均匀分散的 FeP 纳米晶体作为催化剂, 在锂硫电池氧化还原反应中引发快速的 LiPSs 转化。锚定在 rGO-CNT 框架上的 FeP 纳米晶体提供了大量的吸附界面, 促进 Li_2S 成核和生长, 从而增强氧化还原反应动力学。由于 FeP 是一种非活性物质, 在工作电压内过量的材料会降低整体的能量密度, 而吸附和催化只发生在宿主表面, 这意味着构建具有高活性表面的 FeP 架构是必要的。Ma 等[35]通过在溶剂热程序中磷化自组装的海胆状 FeOOH 前体来构建空心海胆 FeP (如图 5(b)), 为 LiPSs 提供更多的活性表面。通过动力学研究进一步证实 FeP 催化 LiPSs 转化的能力, 尤其是从 S_8 向 Li_2S_4 还原的这一过程, 无论是作为硫宿主(如图 5(c-i))还是功能隔膜(如图 5(c-ii)), FeP 的加入都实现了良好的循环稳定性和倍率性能。Xia 等[36]合成了一种由嵌入梯度多孔碳微球中的 FeP 纳米颗粒组成的 Li-S 电池阴极主体 PCM/FeP , FeP 纳米颗粒在梯度多孔导电碳骨架内的均匀分布使活性多硫化锂结合位点和催化位点的最大化暴露成为可能, 从而保证了高催化效率, 确保了高硫利用率。 FeP 对 Li_2S_4 的吸附构型如图 5(d)所示。

此外, 具有不同构成的磷化铁的异质结材料构成了双向催化剂体系, 通过内置电场的调控对多硫化物的吸附进行调节并加速电荷转移。Zhao 等[37]通过简单的硬模版法和磷化, 制得 $\text{FeP}/\text{Fe}_2\text{P}$ 异质结构, 综合了 FeP 的催化能力的和 Fe_2P 的强吸附能力(如图 5(e)), 异质结构中 Fe 3d 和 P 2p 带的键合轨道和反

键轨道之间 d-p 带中心减小(如图 5(f)), 在费米能级上提高的电子浓度增加了其与多硫化锂键合的可能。反应活化能的降低有效加速了锂离子转移速率, 在大电流以及高载量下均具有良好的稳定性。但亚铁磷化物在锂硫电池, 尤其是正极中的应用较少, 磷化铁的低活性缺陷仍有待解决。

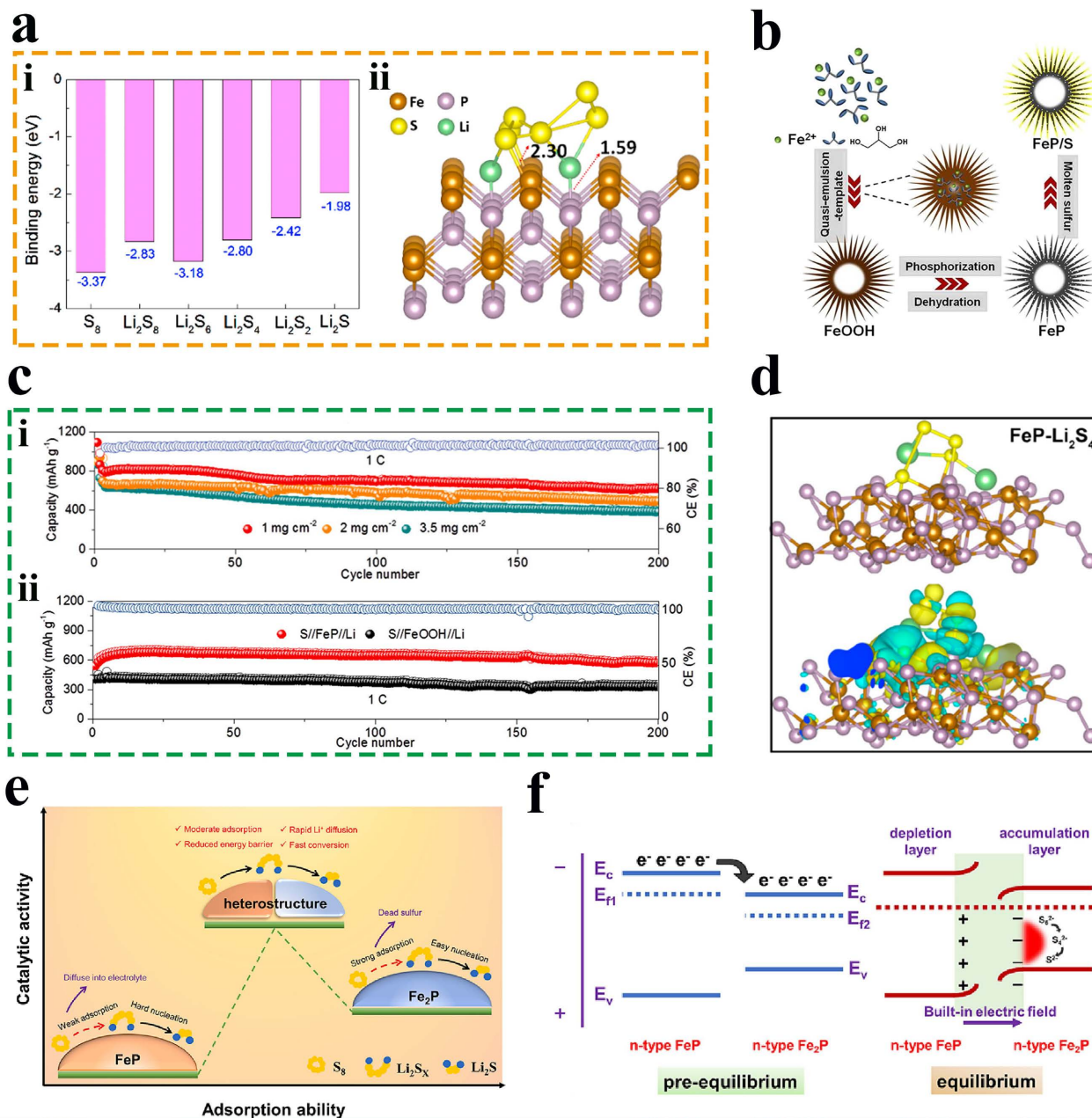


Figure 5. (a) i): Theoretical calculations of binding energies of several sulfur species with the (111) plane of FeP; ii) Geometry of Li_2S_6 binding to the (111) plane of FeP [34]. (b) Preparation diagram of urchin FeP/S [35]. (c) Cycling performances at 1 C of i): FeP/S with various areal S loadings and ii) S//FeP//Li and S//FeOOH//Li [35]. (d) Electronic differential density model of a theoretical model of Li_2S_4 -FeP [33]. (e) The relationship between the adsorption ability and catalytic activity of FeP, Fe_2P and heterostructure and (f) schematic diagrams of the band structure of FeP/ Fe_2P n-n heterostructure before and after contact [37]

图 5. (a) i): FeP 的(111)面对多各硫物种结合能的理论计算; ii): FeP 的(111)面结合 Li_2S_6 的几何结构[34]。 (b) 海胆状 FeP/S 的制备过程[35]。 (c) i): 不同硫面载量的 FeP/和 ii) S//FeP//Li 和 S//FeOOH//Li 电池在 1 C 电流密度下的循环数据[35]。 (d) Li_2S_4 -FeP 的电子差分密度模型[33]。 (e) FeP, Fe_2P 以及异质结构的吸附能力和催化活性之间的关系以及(f) 接触前后 FeP/ Fe_2P 之间 n-n 异质结构的能带结构示意图[37]

2.4. 硫化铁

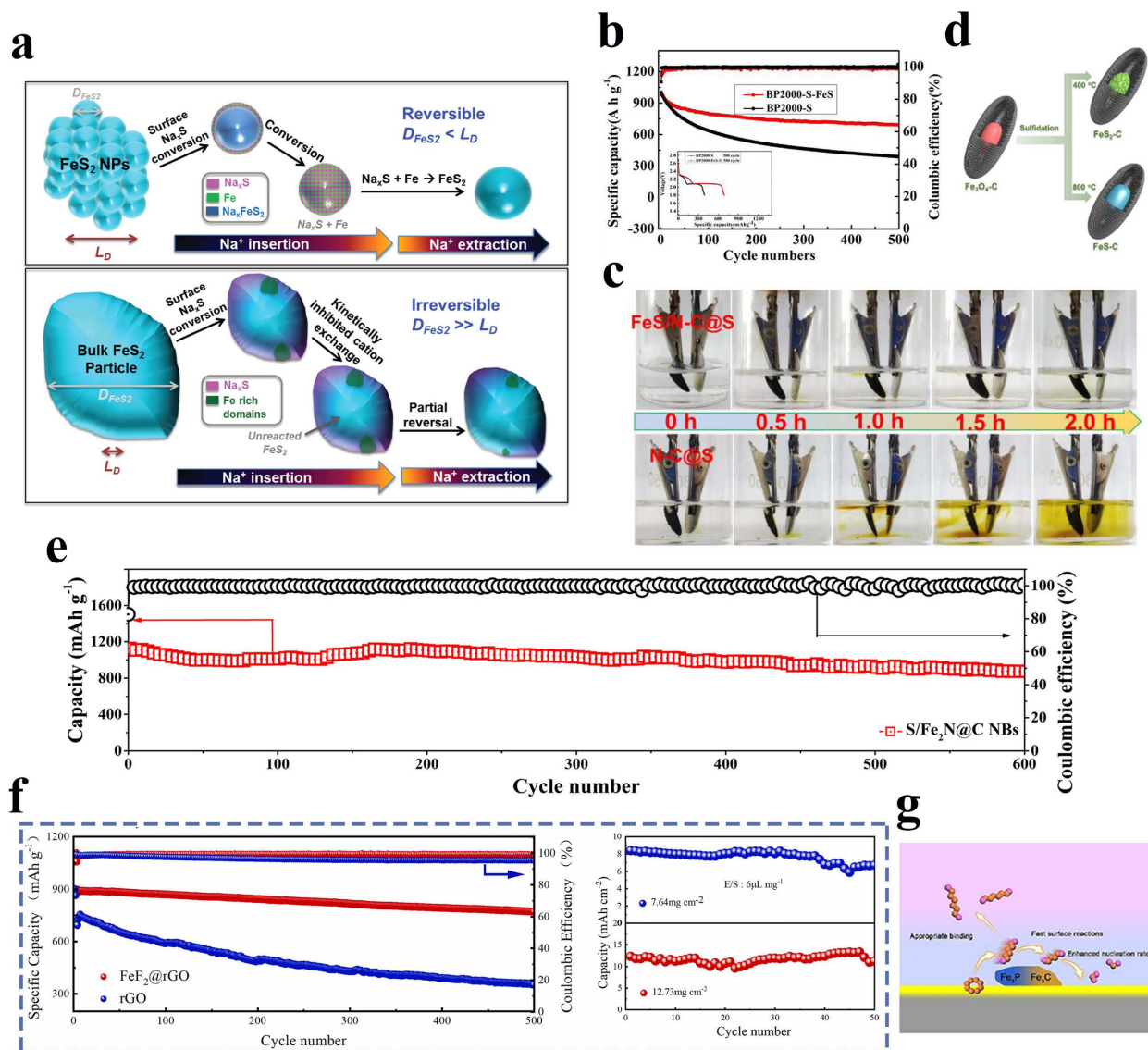


Figure 6. (a) Explanation of the advantages of nanoparticles over bulk FeS_2 in sodium-sulfur batteries [38]. (b) Discharge capacity curves and corresponding Coulombic efficiency of BP2000-S and BP2000-FeS-S composite electrodes in 500 cycles at 0.5 C [45]. (c) Visual confirmation of LiPSs entrapment at the specific discharge of FeS/N-C and N-C cells, both of them discharged at 0.2 C between the open-circuit potential to 1.8 V under identical conditions Schematic illustration of FeS/N-C [49]. (d) Synthetic routes to yolk-shell FeS-C and FeS_2 -C nanospindles [50]. (e) Long-term cycling performance of the S/ Fe_2N @C NBs cathode at 1 C [52]. (f) Cycling performances of FeF_2 @rGO cathode and rGO cathode at 1 C, and under high sulfur loading at 0.1 C [53]. (g) Schematic illustration of synergistic mechanism of Fe_3C - Fe_3P heterostructure [54]

图 6. (a) 在钠硫电池中纳米颗粒比块状 FeS_2 更具优势的说明[38]。 (b) BP2000-S 和 BP2000-FeS-S 复合电极在 0.5 C 电流密度下循环 500 圈的放电比容量曲线以及对应的库伦效率[45]。 (c) 在相同条件下, 在开路电位至 1.8 V 之间以 0.2 C 放电的 FeS/N-C 和 N-C 电池的特定放电中, LiPSs 被捕获的可视观测[49]。 (d) 蛋黄壳 FeS -C 和 FeS_2 -C 的合成路线[50]。 (e) S/ Fe_2N @C NBs 正极在 1 C 下的长循环曲线[52]。 (f) FeF_2 @rGO 和 rGO 正极在 1 C 下的循环, 以及在高硫载量的 0.1 C 下的循环[53]。 (g) Fe_3C - Fe_3P 异质结构的协同作用机理[54]

近年来, 铁基硫化物因良好的导电性、催化性和低成本, 在催化剂和储能器件等领域得到了较多的关注和研究。由于黄铁矿(FeS_2)在自然界含量丰富且低毒性, Douglas 等[38]通过湿法化学合成了一种超

细纳米 FeS_2 纳米颗粒并验证了其良好的储钠/锂的能力。如图 6(a), 通过测试对比不同体积大小的 FeS_2 发现超细颗粒在一定程度上克服了热力学和动力学限制, 为高容量存储和纳米尺寸催化剂[39]的合成开辟了新的途径。Zhang 等[40]通过 EDS 和 Raman 等测试, 结合热力学相图提出多硫化锂(Li_2S_n)与 FeS_2 之间在充放电反应中发生络合, 反应生成 $\text{Li}_2\text{FeS}_{2+n}$ 中间产物达到了吸附 LiPSs 的结果, 这一中间反应减少了活性物质硫的损失。2D 结构、立方结构、核壳结构等[15] [41] [42] [43] [44]不同构型从理论或实验均被证明具有较好的吸附能力和优良的导电性。

差的稳定性导致 FeS 在锂硫电池中应用较少。Yang 等[45]构建了一种填充在 BP2000 孔洞中的 FeS 纳米颗粒(BP2000-FeS), 电子能够从导电 FeS 这一多硫化物的高效吸附剂表面向 Li 转移, 在阻止 LiPSs 转移的同时提供高的放电容量(如图 6(b))。块状[46]和片状[47]的 FeS 均被证明对多硫化物具有优良的锚定能力, 但颗粒间的强物理吸附导致了材料团聚, 不利于长期的循环稳定性。通过简易且成本较低的溶剂热加上高温退火制备得到了碳包覆的纳米花状 FeS (FeS/C)材料[48] [49], FeS/C 独特的花状结构产生了更大的表面来有效的限制多硫化物扩散(如图 6(c)), 降低了电池容量的衰减, 表现出了更稳定的电化学性能, 同时外包的碳层避免了 FeS 在充放电过程中的团聚。这种高效绿色的合成方法使得 FeS/C 有望工业化、规模化生产。不同原子比的硫化铁材料通过简单的温度控制等就可以达成[50] (如图 6(d))。

总的来讲, 由于电池性能一般以及前期电池性能衰减快等问题, 目前对硫化铁的研究依然较少。循环过程中不可抗拒的体积变化和困难的合成方法阻碍了硫化铁的实际应用。当然, 在锂硫电池领域, 越来越多的人致力于探索和开发具有不同形貌和杂化基质的硫化铁材料[51], 以克服这些障碍。

2.5. 其他铁基化合物

除了以上几种常见的化合物, 还有像氮化铁、氟化铁等不常见化合物铁基化合物可用于锂硫电池正极材料。蛋黄核壳结构已经被证实是一种有效的提高锂硫电池性能的结构, Zheng 等[52]成功合成了一种高性价比的多功能 $\text{Fe}_2\text{N}@C$ 蛋黄壳纳米盒($\text{Fe}_2\text{N}@C$ NBs), 极性的 Fe_2N 核对多硫化物的强吸附和有效催化令电池表现出了高可逆容量、出色的倍率性能以及 1 C 下极佳的循环稳定性(如图 6(e))。Sun 等[53]制备了一种氟化铁/石墨烯(FeF_2/rGO)材料作为正极的硫基体, 在充放电反应过程中通过 XRD 等检测出现了 FeF_2 原位转化为 FeS 和 LiF 的现象, LiF 低的扩散势垒实现了高效的离子扩散, 同时 FeS 对多硫化物的强吸附作用协同保障了电池的高效稳定循环。低电化学极化和优异的氧化还原反应动力学保障了在 $12.7 \text{ mg}\cdot\text{cm}^{-2}$ 的高硫负载和 $6 \text{ uL}\cdot\text{mg}^{-1}$ 的贫电解质条件下仍实现了 $12.3 \text{ mAh}\cdot\text{cm}^{-2}$ 的高性能(如图 6(f))。氧化铁、硫化铁的强化学吸附, 碳化铁、磷化铁的导电性和强催化能力等优势突出, 但同时存在的缺陷如氧化铁的弱导电性等也影响了电池性能的进一步提高。异质结构的设计结合了两种材料的优势并有效降低它们的缺陷在电池中的影响(如图 6(g)), 合理的材料搭配为打造更加优良的催化剂提供了合理的策略[54] [55] [56] [57]。

3. 结语

锂硫电池作为替代当下传统储能系统最具实力的竞争者, 高的理论容量吸引了广泛的关注。但存在的多硫化物的穿梭效应、体积膨胀、低导电性等缺陷阻碍了它的稳定高效运行, 解决这些问题是推进锂硫电池工业化的必然要求。铁作为一种最为常见的金属, 不同的铁基化合物所具有的对 LiPSs 独特的化学吸附、快速催化转化、提高电导率等效果, 使得它们作为硫的化学锚和催化活性位点在锂硫电池中具有突出的表现。单一种类铁基材料对锂硫电池性能的改善方式还较为单一, 这就需要研究者们开发合适的异质结组合来有机结合二者之间的优势。如何设计合适的材料搭配和结构构成, 仍然值得我们去发现和研究。如何有效捕获多硫化物和提高正极导电性仍是目前的研究重点。合适的吸附能力才能够在抑制

穿梭效应的前提下保障活性物质的快速转化；合适的碳基底可以帮助提供大量的储硫空间，设计合适的能够大量制备的金属化合物/碳材料结构是工业化生产的重要前提；此外，能否用于高载量电池、固态电池等也是需要考虑的。锂硫电池工业化的道路还需要研究者的大量投入，正极材料、隔膜、电解质以及锂负极等各部分的研究都是必不可少的，铁基材料在其中拥有着它的一席之地。

项目基金

广西自然科学基金(2022GXNSFAA035463)。

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