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二维半导体异质结光催化分解水制氢研究

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摘　要:日益严重的环境污染和能源紧缺问题使人们开始研究可有效水解析氢的光催化剂。其中二维(2D)半导体光催化剂因其出众的比表面积而极具应用前景。为了克服光生电荷寿命短的关键问题,2D 范德华(vdW)半导体异质结因其作为光催化剂时所展现的分离光生电子和空穴的强大能力而被广泛研究。总结了以 vdW 异质结为代表的 2D 水分解制氢光催化剂的最新研究。在论证了光催化水分解的氧化还原反应的基本原理之后,讨论了许多具有代表性的 2D vdW 异质结,并从理论与实验角度突出了基于过渡金属二卤化物(TMDs)和磷烯异质结作为光催化剂的研究及该研究领域中的机遇与挑战。介绍了 2D vdW 异质结在光催化剂中的应用,为提高水分解产生氢的效率提供了新的思路。

关键词:二维材料;异质结;光催化剂;水分解

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Recent Study of Photocatalytic Water Splitting for Hydrogen Generation Based on Two-dimensional Semiconductor Heterostructure

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Abstract: Due to increasingly serious environmental pollution, people are forced to explore efficient photocatalysts used to decompose water for hydrogen generation. Two-dimensional (2D) semiconductor photocatalyst holds the significant promise because of its novel physical and chemical properties, compared with bulk photocatalyst. To overcome the crucial problem of short lifetime for the photogenerated charges, 2D van der Waals (vdW) heterostructures are used to be formed as a photocatalyst due to the awesome ability to separate the photogenerated electron-hole pairs. The recent development of 2D photocatalyst is reviewed, especially vdW heterostructure photocatalyst for water splitting. After demonstrating the fundamentals of light-driven redox reaction for water splitting, this paper makes a study of the transition metal dichalcogenides (TMDs) and phosphorus from theory and experiment in the highlight, which are used as heterostructure photocatalyst, introduces the application of 2D vdW heterostructure photocatalyst and discusses its opportunities and challenges.

Keywords: two-dimensional materials; heterostructure; photocatalyst; water splitting

0　引言

由于全世界化石燃料的使用引起全球气候变化,使近几十年来能源和环境问题变得越来越严重[1-2]。为了解决这些问题,开发清洁能源材料变得至关重要[3]。氢气(H_2)是一种非常具有前景的新能源,其燃烧时的唯一产物就是水,故被认为是一种绿色、可持续的能源[4-5]。因此,很多研究者已经开发了一些制氢方式,如:聚合物膜(PEM)水电解[6]、乙醇蒸汽重整[7]、热化学分解[8]、光电解[9-10]和光催化[4,11-12]等。其中,因为太阳能具有高能量但低利用率[13-14],使 H_2 的光催化分解水方法极具研究价值。利用催化剂来吸收太阳能促发水的氧化还原反应,使得水分解出氢气的过程揭示了光催化剂的重要作用。

在最近研究中,单原子层材料石墨烯是材料科学和凝聚态物理中的后起之秀[15]。这种 2D 材料由于高的比表面积,具有非常新颖的物理和化学特性[16]。石墨烯在电子、光电、光伏和传感中的应用特别广泛[17]。但是,石墨烯是带隙为零的半金属材料,因此不适合诸如场效应晶体管的应用[18]。与此同时,过渡金属二卤化碳(TMDs)[19]、磷稀[20]、砷稀[21]等诸多 2D 半导体材料也引起了人们研究兴趣,这些 2D 材料都具有优异的电子[22-24]、热学[25-28]、磁学[29-32]、热电[33-35]以及光学[36-41]性质。同时,这些性质都能被外应力[42-44]、掺杂[45-47]、吸附[48-51]、缺陷[52-55]以及结构[56-59]调节等方式调控,这也使其在光催化[60-61]、光电极[62]、光探测器[63]、PN 结[64]的应用具有非常大的前景。到目前为止,研究者们已经开发了很多方

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法来控制层状材料的几何形状和尺寸。例如固溶相的生长提供了一种简单的生产方法,可用合成具有精确厚度和基本尺寸的 2D 材料。该方法可用于生成 TiS_2 纳米片,如图 1 所示[65]。图 1(a)和图 1(b)为低分辨率 TiS_2 层的 TEM 图像,图 1(a)中的插图为多层 TiS_2 纳米片的图像;图 1(b)中的插图是单层 TiS_2 区域的电子衍射图;图 1(c)和图 1(d)是高分辨率 TEM 图像,展示了单个 TiS_2 层的边缘和底面[66]。

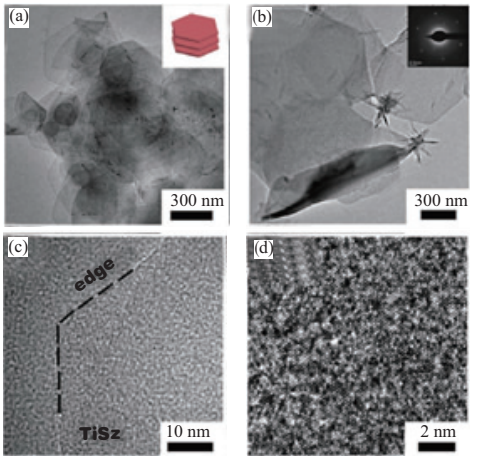


图 1　TiS_2的表征图

为了扩展单层半导体材料的应用,研究者开始创建半导体异质结,这不仅保留了原始单层材料的特性,而且还提供了其他迷人的性能[67]。此外,许多 2D 晶体材料已经通过实验合成了,而且可以通过 vdW 代替共价相互作用来构建各种异质结。例如,MoS_2/石墨烯/ WSe_2vdW 异质结可用于光检测,如图 2(a)所示。MoS_2/石墨烯/ WSe_2 vdW 异质结的光学图像见图 2(b)上图,示意性侧视图见图 2(b)下图。图 2(c)显示了用于光检测异质结的光学显微镜图像,其中黄色、灰色和绿色线分别显示了 MoS_2、石墨烯和 WSe_2(本刊为黑白印刷,有关疑问咨询作者)。这个异质结还具有出色的器件性能。例如,在近红外光区域的比探测率约为 10^{11} Jones,如图 2(d)所示。图 2(e)和图 2(f)分别是 MoS_2/石墨烯/WSe_2 vdW 异质结在 V_{ds} = 0 和 V_{ds} = 1 V 时的光电流映射光电流映射[68]。

大量研究表明,2D 材料作为光催化剂将水分解为 H_2 和 O_2,相比于块体材料具有明显的优势。与块体光催化剂相比,2D 材料的极大比表面积为光生电荷到表面进行氧化还原反应提供了非常短的迁移路径。本文简要介绍了不同类型异质结的形成,概括了半导体作为光催化剂分解水的基本原理,解释了 2D 半导体异质结作为光驱动催化剂分解水的优势。在介绍一些代表性 2D vdW 异质结的最新研究时,重点集中于材料的结构、电子、界面和光学性质,以进行光催化整体水分解性能的探讨。最后,对 2D 材料作为光催化剂分解水制氢的研究进行系统地总结和展望。

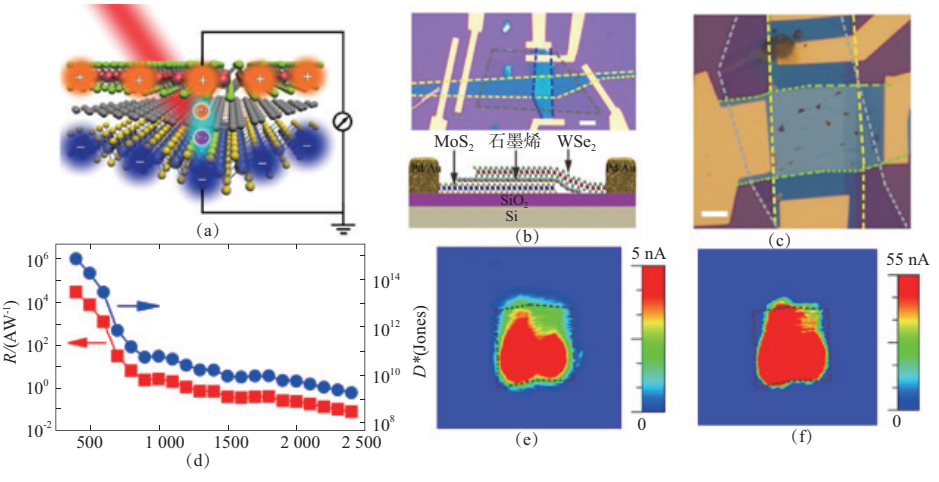


图 2　MoS_2/石墨烯/WSe_2异质结的应用、表征与性能

1　不同类型异质结的合成

考虑到两种材料的能带边缘位置,将半导体异质结分为 3 种类型,即 I 型、II 型和 III 型。当异质结由半导体 A 和半导体 B 堆叠时,如图 3(a)所示。如果两个半导体的导带最小值(CBM)和价带最大值(VBM)都遵循以下关系:$CBM_B > CBM_A > VBM_A > VBM_B$,那么就形成 I 型异质结;因为异质结的 VBM 和 CBM 都由半导体 A 贡献,所以光生电子和空穴很容易复合,这意味着它不适合用作光催化剂。如图 3(b)所示,II 型异质结是交错带结构,遵循 $CBM_A > CBM_B > VBM_A > VBM_B$,这样的 II 型异质结可以将光生电子和空穴分离到不同的层,因此有望用于光催化剂[69-70]。III 型异质结的能带结构具有 $CBM_B > VBM_B > CBM_A > VBM_A$的特性,如图 3(c)所示。这种 III 型异质结构可用于隧穿场效应晶体管[71]。

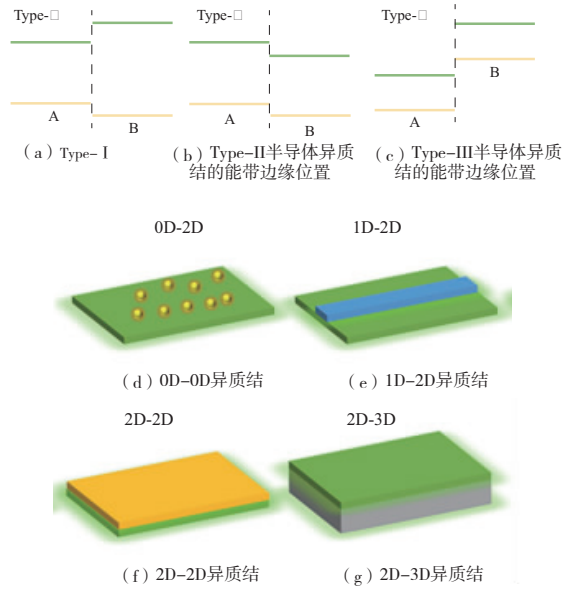
根据材料的尺寸,vdW 异质结可以分别分为 0D-2D、1D-2D、2D-2D 和 2D-3D 异质结。对于 0D-2D vdW 异质结,0D 材料通常是量子点,如图 3(d)所示。典型的 0D-2D vdW 异质结可以通过水热法与微乳液制备,如 g-C_3N_4/MoS_2显示出优异的光催化氧化还原性能[72]。纳米棒和纳米线结构可用于实现 1D-2D vdW 异质结(图 3(e)),TiO_2/CdS 异质结显示出优异的光生载流子分离效率和电子转移能力[73]。化学气相沉积(CVD)方法用于生长 Bi_2S_3/MoS_2异质结,该异质结在

光电子器件(如场效应晶体管和光电探测器)中具有广阔的应用前景[74]。XIAO R 等人基于过渡金属碳化物(MXene)合成了 CdS/Ti_3C_2异质结,这种肖特基异质结可作为光催化剂分解水生成 H_2,在氢释放反应中显示出优异的性能,约为 2 407 μmol·g^{-1}·h^{-1}[75]。其他一些研究的异质结氢气生产能力如表 1 所示。

表 1　部分异质结作为光催化剂时的制氢效率

光催化剂	光源	制氢效率/(μmol·g^{-1}·h^{-1})	文献
CdS/Ti_3C_2	300 W Xe 灯	2 407	[75]
g-C_3N_4/NiAl	300W 石英钨卤素灯	3 170	[76]
g-C_3N_4/SnS_2	300 W Xe 灯	972.6	[77]
Cu/TiO_2@$Ti_3C_2T_x$	500 W Xe 灯	860	[78]
CdS/WO_3	500 WXe 灯	2 900	[79]
g-C_3N_4/NiFe	125 W Hg 灯	1 488	[80]
CdS/Ni-Fe	300 W Xe 灯	469	[81]
CdSe/ZnCr	300 W Xe 灯	2 196	[82]
Cu_2O/ZnCr	300 W Hg 灯	3.42	[83]

大量研究还探索了 2D-2D 异质结的合成方法和出色的性能(图 3(f))。例如,P-$La_2Ti_2O_7$/Bi_2WO_6[84]、Cu_2S/$Zn_{0.67}Cd_{0.33}S$[85]、TiO_2/g-C_3N_4[86]、$FeSe_2$/g-C_3N_4[87]等。如图 3(g)所示,2D-3D vdW 异质结由于其具有 2D 材料的新颖特性和 3D 材料的稳定性,也引起了广泛的关注。一些理论和实验研究表明 2D-3D vdW 异质结可用于光催化,光电和纳米电子器件,例如 MoS_2/Si[88]、MoS_2/MoO_2[89]、MoS_2/GaN[90]和 WS_2/Si[91]。2D vdW 异质结比单独的单层材料提供了更有希望的应用,并具有改进的氧化还原性能,可以分解水以生产 H_2[92]。



(a) Type-I　(b) Type-II半导体异质结的能带边缘位置　(c) Type-III半导体异质结的能带边缘位置

(d) 0D-0D异质结　(e) 1D-2D异质结　(f) 2D-2D异质结　(g) 2D-3D异质结

图 3　不同异质结的分类

2　光催化分解水的基本原理

光催化分解水的基本原理简要说明如下。在图 4(a)中,被光照射的单层半导体吸收了大量的光子能量,光子产生的电子将转移到半导体光催化剂的导带(CB),并且光子产生的空穴保留在价带(VB)中。半导体能带边缘的合适能级对于决定光子产生的电子-空穴对的还原和氧化性能非常重要。作为一个合理的半导体光催化剂,CBM 的势能应该比水分解的还原电位 H^+/H_2(-4.44 eV)更高,而 VBM 应该比水分解的氧化电位更负,即 O_2/H_2O(-5.67 eV)。因此,对发生整体水分解的氢气分解反应(HER)和氧气分解反应(OER)的表达式如下所示:

$$\text{氧化反应：}H_2O+2h^+ \rightarrow 2H^+ + 1/2O_2 \quad (1)$$

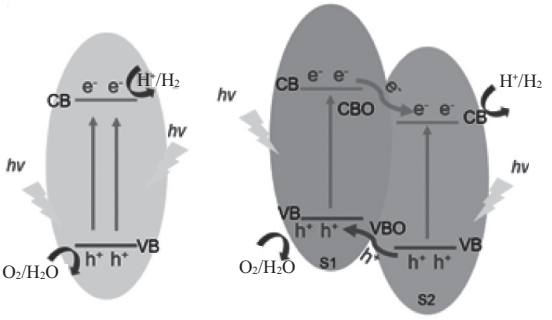
$$\text{还原反应：}2H^+ + 2e^- \rightarrow H_2 \quad (2)$$

$$\text{总反应：}H_2O \rightarrow H_2 + 1/2O_2 \quad (3)$$

此外,上述水分解中的还原和氧化电势是在 pH=0 的条件下的。对于非零的 pH 值,它们变为[93]:

$$E^{red} = -4.44\ eV + pH \times 0.059\ eV \quad (4)$$

$$E^{oxd} = -5.67\ eV + pH \times 0.059\ eV \quad (5)$$



(a) 单层半导体　(b) 2D半导体异质结

图 4　单层和 2D 异质结为光催化剂分解水的示意图

3　2D 异质结光催化分解水

3.1　异质结作为光催化剂的优势

当半导体单层用作分解水的光催化剂时,CB 处光子产生的电子和 VB 处光子产生的空穴迅速结合并通过热或光消耗能量[94]。这导致激发态电子的寿命非常短,仅为 3~10 ps,而载流子扩散时长仅为 2~4 nm[95]。此外,由于催化剂中可以俘获电子或空穴的晶体缺陷,因此更容易发生光子产生的电子与空穴的复合。因此,至关重要的是,探索一种分离光子产生的电子和空穴以延长光催化剂寿命的策略。

最常用一种策略是堆叠两个不同的层(S1 和 S2)材料,以构造具有 II 型的 2D vdW 异质结,如图 4(b)所示。vdW 异质结吸收光能后,电子和空穴在 CB 和 VB 处被激发。在 S1 的 CB 处光生电子将在导带偏移(CBO)的帮助下转移至 S2 的 CB,并且光生空穴将从 S2 的 VB 移至 S1 的 VB,这意味着光生电子与空穴的复合得到了有效抑制。因此,延长光生电荷载流子的寿命,并可以分别提高 HER 和 OER 的效率。作为促进光生电子-空穴对在两层之间迁移的一种激发力,研究者通过基于密度泛函理论(DFT)的 Heyde-scuseriae-ernzerhof(HSE06)计算研究得到了一些 II 型 vdW 异质结的 CBO 和 VBO 如表 2 所示。

表 2　vdW 异质结光催化剂中的能带偏移

光催化剂	CBO/eV	VBO/eV	文献
$MoS_2/Mg(OH)_2$	3.21	0.46	[96]
$WS_2/Mg(OH)_2$	1.94	0.17	[96]
MoS_2/ZnO	2.49	0.58	[97]
WS_2/ZnO	2.00	0.26	[23]
$MoSe_2/BP$	0.55	0.03	[37]
g-GaN/BSe	0.16	0.35	[60]

近年来,基于 2D vdW 异质结的高效光催化剂分解水性能已得到广泛的研究。具有 II 型能带结构的 vdW 异质结不仅可以分隔光子产生的电子和空穴,还具有不错的吉布自由能[98]、激子结合能[99]、载流子迁移率[69, 100]和光吸收性能[101-102]等。详细地讲,引起还原反应的 g-GaN/$Mg(OH)_2$ vdW 异质结的吉布自由能差低至-0.475 eV,显示出优异的 HER 中的催化性能[98]。与原始 C_2N 和 WS_2 单层相比,C_2N/WS_2 vdW 异质结可以显著降低激子结合能,如图 5 所示,这更有利于光子产生的电子-空穴对的分离[99]。此外, vdW 异质结可以通过界面耦合[103]、外应力[60, 104]和外电场[105-106]调节其各方面性质。例如,图 6 显示了在不同外部双轴应变下 ZnO/GaN vdW 异质结能带边缘位置的能级[70]。下面主要介绍基于典型 2D 材料(包括 TMDs 和磷)异质结的研究,并展示它们如何充当分解水的优异光催化剂。

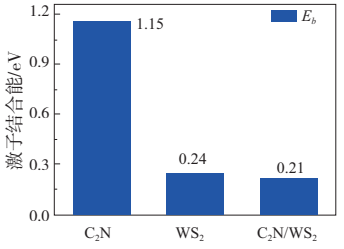


图 5　C_2N、WS_2和 C_2N/WS_2 vdW 异质结的激子结合能

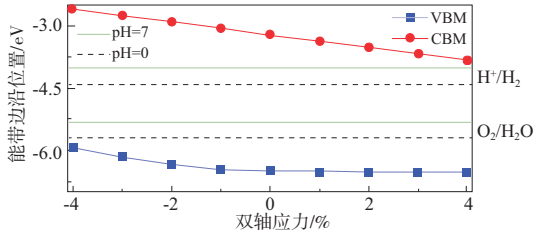


图 6　ZnO/GaN vdW 异质结在 pH=0 和 pH=7 时用于光催化水分解的可调电子性能

3.2　基于 TMDs 的异质结光催化剂

TMDs 材料通常定义为 MX_2(M = W,Mo;X = S,Se),由于其迷人的电子和热电性能而备受关注[107-108]。同时,TMDs 的可制造性也使其成为新兴纳米材料的焦点[109-112]。用 CVD 法合成的 MoS_2 和 h-BN 的垂直 vdW 异质结,可以显著提高光吸收性能[113]。MoS_2/CdS 异质结是通过一锅溶剂热过程产生的,并且在可见光照射下产生了惊人的 H_2生成能力(大约 137 $\mu mol h^{-1}$)[114]。用金纳米颗粒修饰的 MoS_2和 WS_2的异质结表现出强大的 HER 能力,因为金纳米颗粒的沉积非常均匀且致密[115]。MoS_2/WSe_2 vdW 异质结也被证明了具有 II 型能带排列结构[116]。

基于 TMDs 的 vdW 异质结具有交错带结构,例如 MoS_2/ZnO 和 WS_2/ZnO[23]、g-GaN/MoS_2 和 g-GaN/WS_2[22]、$MoS_2/Mg(OH)_2$和 $WS_2/Mg(OH)_2$[96]、MoS_2/BSe 和 WS_2/BSe[117]、$MoSe_2$/BP 和 WSe_2/BP[37]等。这些基于 TMDs 的 vdW 异质结都具有防止光子产生的电子与空穴复合的能力。一些学者通过 HSE06 计算方法研究了基于 TMDs 的 vdW 异质结的能带排列[118],得到了基于 TMDs 的 vdW 异质结的能带边缘位置,与分别在 pH=0(红色线标记)和 pH=7(紫色线标记)时分解水的氧化能级(O_2/H_2O,用实线表示)和还原能级(H^+/H_2,用虚线表示)进行了比较(红线标记)[22, 96, 97, 117](图 7)。基于第一性原理[119],说明这些基于 TMDs 的异质结的 CBM 和 VBM 的能量位置在适当的 pH 值下对于促进水分解的氧化和还原是可行的。

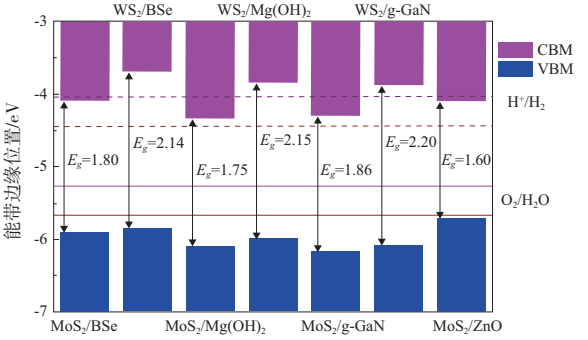


图 7　异质结的能带边缘位置图

ZHANG J 等通过控制单层 $MoSe_2$的硫化来合成 TMDs 材料,该单层 $MoSe_2$被 S 原子取代了顶层的 Se 原子。(图 8(a)为 Janus MoSSe 单层的顶视图和侧视图,黄色、绿色和橙色球体分别表示 Mo、S 和 Se 原子,称为 Janus TMDs[120]。图 8(b)-图 8(g)分别显示了 Janus MoSSe 的光学图像拉曼光谱、PL 峰强度图、AFM 形貌和 HRTEM 图像、区域电子衍射图。ZHANG J 等还使用密度泛函理论来研究这种特殊的不对称结构导致的高碱表面析氢反应性能。LU A Y 等[121]报道了具有较大平面外压电极化的 Janus TMD,多层 Janus MoSTe 约为 5.7~13.5 pm/V,其键合电荷密度如图 8(h)所示,并证明了此 Janus TMD 具有压电潜力[122]。Janus TMD 还具有较长的激发载流子寿命,约为 2 ns,如图 8(i)所示,与基于 TMD 的异质结构相当[100]。除了 Janus MoSSe,其他 Janus TMD(MoSTe,MoSeTe 等)也具有明显的电子特性(带隙在 1.37~1.96 eV 之内)和高载流子迁移率[123],如图 8(j)所示(300 K 时,上图为电子迁移率,下图为空穴迁移率)。而且,Janus TMDs 材料具有很高的光吸收能力[124-125],并具有适当的能带边缘位置以促进氧化还原反应(图 8(k)),填充直方图和阴影直方图分别显示了沿 armchair 和 zigzag 方向的载流子迁移率[123]。所有这些研究都表明 Janus TMDs 是有希望的光催化剂。同时,许多研究也证明了基于 Janus TMD 的 vdW 异质结作为光催化剂分解水的可行性,例如 MoSSe/

WSSe[126]、MoXY (X/Y = O, S, Se, 和 Te; X ≠ Y)[127]、MoSSe/WSe_2[128] vdW 异质结, 这些都可以作为出色的光催化剂分解水。

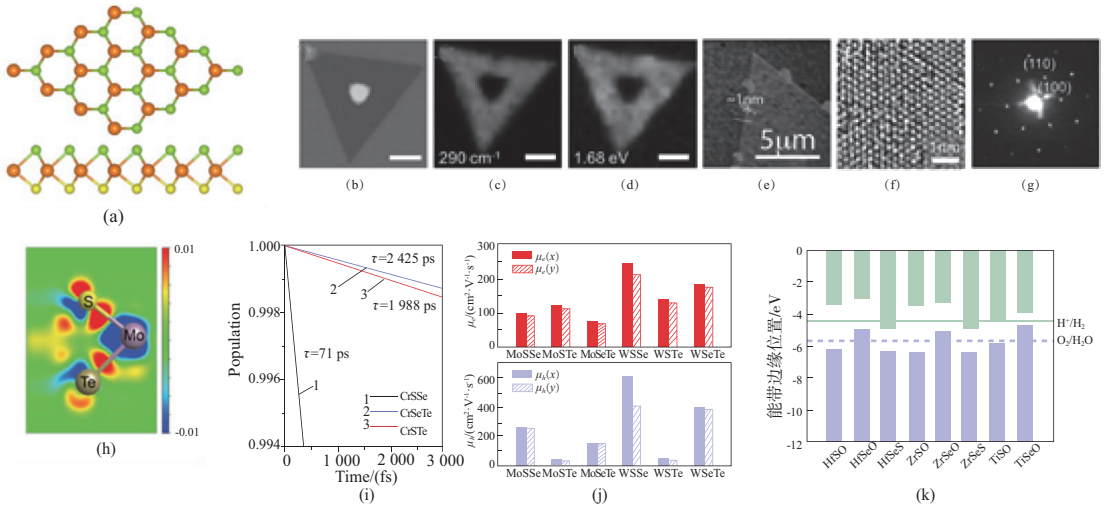


图 8　基于 TMDs 材料的特性

列举两种基于 Janus MoSSe 的代表性 vdW 异质结,即 MoSSe/GaN 和 MoSSe/AlN[130]。MoSSe/GaN 和 MoSSe/AlN vdW 异质结的动态和热稳定性分别通过分子动力学声子谱和(AIMD)模拟计算来证明,如图 9(a)-图 9(d)所示。图 9(e)和图 9(f)分别描述了 MoSSe/GaN 和 MoSSe/AlN vdW 异质结的投影能带结构(灰色虚线表示费米能级,并设置为 0)。显然,MoSSe/GaN(MoSSe/AlN) vdW 异质结的 CBM 和 VBM 分别由 MoSSe 和 GaN(AlN)层贡献。因此,两个 vdW 异质结都具有典型的 II 型能带结构。因此,它将光子产生的电子和空穴分别分离到 MoSSe 和 GaN(AlN)层。MoSSe/GaN 和 MoSSe/AlN vdW 异质结的电子定位功能(ELF)分别如图 9(g)和图 9(h)所示。图 9(i)展示了 MoSSe/GaN 和 MoSSe/AlN vdW 异质结均具有适当的势能,可用于水在 pH = 0 时分解的氧化还原反应。此外,计算的 MoSSe/GaN(MoSSe/AlN) vdW 异质结的载流子迁移率(图 9(j))表明,基于 Janus MoSSe 的 vdW 异质结均可提高载流子迁移率。因此,MoSSe/XN(X = Ga, Al) vdW 异质结具有潜在的高效光催化水分解能力。

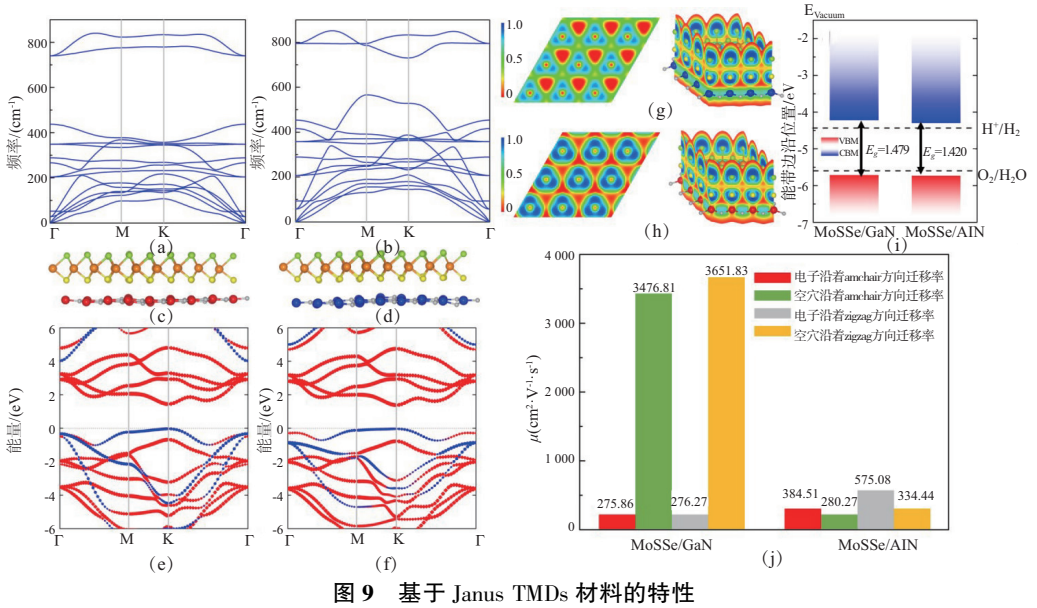


图 9　基于 Janus TMDs 材料的特性

3.3　基于磷烯的异质结光催化剂

除 TMDs 材料外,磷烯、蓝磷(BlueP)和黑磷(BlackP),也引起了研究学者广泛关注。BlackP 和 BlueP 可以通过外延生长实验合成和调制等离子体处理,图 10(a)和图 10(b)分别为 Au(111)上单层磷的 STM 图像[131]和 BlackP 的 TEM 图像[132]。BlackP 拥有优越的电子[133-135]、热学[136-138]、光电[139]、光学[38, 140, 141]性质以及高载流子迁移率[142],这使得 BlackP 可用于锂离子电池[143]、异质结[144]、场效应晶体管[145]和光电器件[146]。

与 BlackP 的褶皱蜂窝结构不同的是,BlueP 具有六角形蜂窝结构。图 10(c)为掺杂 B、C、N、O 和 F 的 BlueP 系统的电子结构和非键合状态演化的示意图。B 掺杂的 BlueP 显示直接带隙,并且在 C 掺杂和 O 掺杂的系统中可

观察到自旋极化现象,这使得 BlueP 有望应用在光学和自旋电子器件中[147]。当 vdW 异质结由 BlueP 构造时,它还会触发一些可调的界面属性[103]。BlueP/MS_2(M = Nb,Ta) vdW 异质结显示出改善的电导率和增强的机械柔韧性(最终应变> 17%)[148]。此外,通过对锂吸附系统的研究(如图 10(d)所示),BlueP/NbS_2 vdW 异质结的高容量(约528.257 $mAhg^{-1}$)表明其具有作为电极的应用潜力。图 10(e)为 BlueP/NbS_2和 BlueP/TaS_2 vdW 异质结的比容量。

当 vdW 异质结由 g-GaN 和 BlueP 单层堆叠时,除了 CBO 和 VBO 以外,由能带弯曲产生的界面附近的内置电场也可以分离光子产生的电子和空穴[42],图 10(f)为在 g-GaN/BlueP vdW 异质结的界面附近形成能带弯曲。一些研究表明,BlueP/TMDs (BlueP/MoS_2、BlueP/WS_2、BlueP/$MoSe_2$和 BlueP/WSe_2) vdW 异质结具有出色的电子性能和吸收可见光的能力[149]。所有这些结果都证明基于磷烯的 vdW 异质结用作光催化剂是非常有前途的。

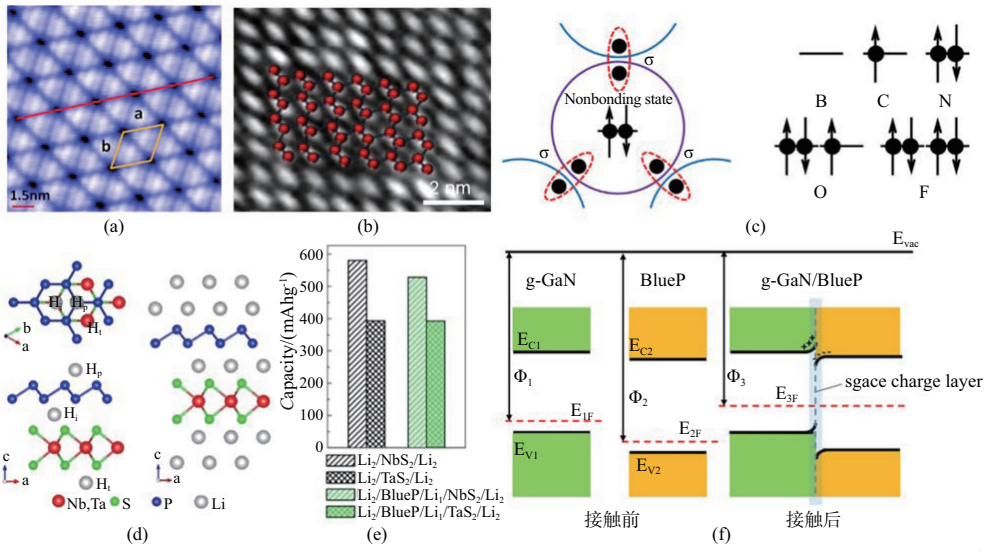


图 10　磷烯材料的基本特性

已有研究证明,BlueP/XC(X = Ge 和 Si)异质结是通过 vdW 力形成的,并且两个异质结均具有 II 型能带结构,如图 11(a)和图 11(b)所示[150](黑色和红色标记分别是 BlueP 和 GeC(SiC)层的能带贡献;灰色虚线表示费米能级,其设置为 0)。从投影能带结构和态密度(DOS)计算中可以看到 BlueP/GeC(BlueP/SiC) vdW 异质结的 CBM 和 VBM 由 BlueP 和 GeC(SiC)层贡献,这意味着光生电子-空穴将被分离,并分别运动到 BlueP 和 GeC(SiC)层促使 HER 和 OER。有趣的是,BlueP/GeC vdW 异质结可以诱导 pH=7 时水分解中的氧化还原反应,而 BlueP/SiC vdW 异质结具有诱导 pH=0 的环境下水分解的 HER 和 OER 的能力图 11(c)。同时,沿着 BlueP/GeC 和 BlueP/SiC vdW 异质结的真空层,其电位有一个明显的差降 ΔV,如图 11(d)和图 11(e)所示,这可能导致较大的内置电场进一步分离光生电子-空穴对。更重要的是,与 BlueP、GeC 和 SiC 单层相比,BlueP/GeC 和 BlueP/SiC vdW 异质结甚至可以改善可见光谱区域的吸收,如图 11(f)所示。因此,基于 BlueP 的 vdW 异质结也是可用于水分解的有前途的有效光催化剂。

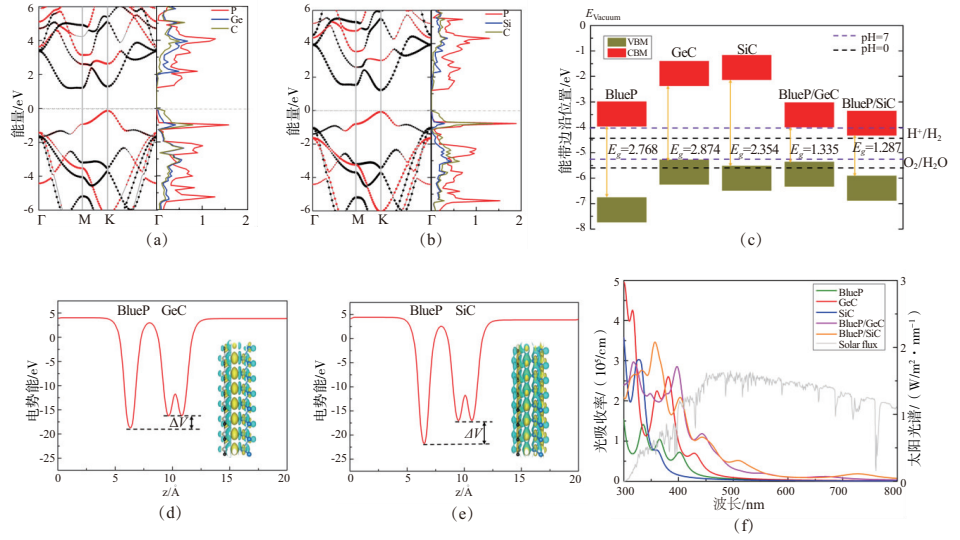


图 11　基于 BlueP 的异质结特性

4　结语

综上所述,本文介绍了用于产生氢气的 2D vdW 异质结光催化剂研究的最新进展,包括:1)光驱动单层半导体的思路可作为水分解用光催化剂的基本原理;2)2D vdW 异质结相对于单层材料作光催化剂分解水更具优势;3)vdW 异质结在水分解方面还有一些优越性能,例如吉布斯(Gibb's)自由能、激子结合能和较长的光生电荷寿命等。此外,还介绍了有关基于 TMDs 和 BlueP 的 vdW 异质结作为光催化剂在水中诱导 HER 和 OER 的最新研究成果。显然,该领域的进展表明可以通过形成 2D vdW 异质结来提高水分解的光催化效率。

到目前为止,研究者们已经证实,2D vdW 异质结可通过吸收太阳能来分离光生电子和空穴,并进一步促使水发生氧化还原反应的能力。尽管某些研究已初见成效,但对于整体性能仍然具有挑战性。在理论与实验相结合的研究中,仍然存在许多未决的问题和挑战。例如,2D vdW 异质结在不同 pH 水溶液环境中的稳定性。此外,即使某些 vdW 异质结具有出色的光吸收性能,也需要系统研究来了解太阳能到氢(STH)的转化效率,以便进一步提高光学性能。最近,由于具备了实验和计算产生的大数据,机器学习方法已被用于各种功能材料的发现[151-152]。期待机器学习方法可以促进光催化剂的开发。相信 2D vdW 异质结对水的分解研究仍然是一个热门的课题,希望本文可以为其未来发展提供一些启发。

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