**Preparation of MoS$_2$–MoO$_3$ Hybrid Nanomaterials for Light-Emitting Diodes**

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Abstract: A facile strategy to prepare MoS$_2$–MoO$_3$ hybrid nanomaterials is developed, based on the heat-assisted partial oxidation of lithium-exfoliated MoS$_2$ nanosheets in air followed by thermal-annealing-driven crystallization. The obtained MoS$_2$–MoO$_3$ hybrid nanomaterial exhibits p-type conductivity. As a proof-of-concept application, an n-type SiC/p-type MoS$_2$–MoO$_3$ heterojunction is used as the active layer for light-emitting diodes. The origins of the electroluminescence from the device are theoretically investigated. This facile synthesis and application of hybrid nanomaterials opens up avenues to develop new advanced materials for various functional applications, such as in electronics, optoelectronics, clean energy, and information storage.

Ultrathin layered MoS$_2$ nanosheets have been widely studied recently because of their unique physical, electrical, and optical properties.[1] To prepare ultrathin MoS$_2$ nanosheets, many methods have been developed, which include mechanical exfoliation,[2] solvent exfoliation,[3] lithium intercalation,[4] and chemical vapor deposition.[5] In particular, the characteristics of 2D MoS$_2$ nanosheets have been intensively investigated. For example, its electrocatalytic activity for hydrogen production has been found to be only slightly lower than that of the precious platinum noble metals and thus surpasses most common metals, which might arise from the large number of active edge-sites on MoS$_2$.[6] Additionally, as the channel of field-effect transistors (FETs), the single-layer MoS$_2$-based top-gated FET exhibited ultra-high channel mobility (approximately 200 cm$^2$V$^{-1}$s$^{-1}$) and a current on/off ratio of approximately 10$^8$[7] These results enable single-layer MoS$_2$ to be a competitive candidate for potential replacement of silicon in CMOS-like logic devices (CMOS = complementary metal–oxide semiconductor).[2,3,4b,8] Furthermore, the quantum enhancement in the photoluminescence (PL) intensity from a few layers to a single layer can be measured in both mechanically[9] and chemically[10] exfoliated MoS$_2$ nanosheets. Impressively, single-layer MoS$_2$-based phototransistors with high photoresponsivity[10a,b] and diodes with excellent electroluminescence (EL)[10c,d] have been reported.

As an important class of materials, 2D hybrid nanostructures are attracting intense interest. For instance, the vertically layered heterostructured FETs, that is, graphene/BN/graphene[11] and graphene/WS$_2$/graphene[12] prepared by the dry-transfer technique, exhibited field-effect vertical-tunneling characteristics. The FETs based on n-MoS$_2$/graphene and n-MoS$_2$/graphene/p-Bi$_2$Sr$_2$Co$_2$O$_8$/graphene vertical heterostructures showed the functional properties of logic transistors and complementary inverters.[13] The layered MoS$_2$/graphene composite, synthesized by the solvothermal method, was used as an anode material for a lithium-ion battery with excellent electrochemical performance.[14] The layered nanojunction of MoS$_2$/CN, synthesized by wet impregnation followed by thermal-assisted sulfidation, showed excellent photocatalysis for H$_2$ evolution.[15] Moreover, the Van der Waals heterostructures of WS$_2$/MoS$_2$ were recently studied for exploration of the EL and photocurrent generation properties.[16]

Herein, we demonstrate a facile method to prepare MoS$_2$–MoO$_3$ hybrid nanomaterials. The preparation is achieved through the in situ partial oxidation of MoS$_2$ nanosheets during their film preparation by a heat-assisted spray-coating procedure in air, followed by thermal-annealing-driven crystallization. After spray coating the obtained MoS$_2$–O$_x$ film on an arbitrary solid substrate, such as Si, SiC, quartz, or glass, the material undergoes thermal treatment and crystallizes to form MoS$_2$–MoO$_3$ hybrid nanomaterials composed of (001)-dominated MoS$_2$ and (002)-dominated α-MoO$_3$. The obtained MoS$_2$–MoO$_3$ nanomaterial exhibits...
p-type conductivity. As a proof-of-concept, a light-emitting diode (LED) is demonstrated, which is based on a heterojunction composed of a p-type MoS$_2$–MoO$_3$ (p-MoS$_2$–MoO$_3$) film and an n-type 4H-SiC (n-SiC) substrate, and exhibits multi-wavelength emission. Two bands in its EL spectrum are assigned to the internal radiative recombination of electrons from the conduction band (CB) and holes from the valence band (VB) of MoS$_2$, and that of electrons from the CB and holes from the VB of MoO$_3$, respectively. The other two bands were correlated to the defect energy levels in MoO$_3$ supported by theoretical calculations.

In a typical experiment (see Experimental Section for further details), the lithium-exfoliated MoS$_2$ nanosheets, prepared by our recently developed method,[4a] were first sonicated in a water bath (Figure 1a). Field-emission scanning electron microscopy (FE-SEM) images in Figure 2a show that the lateral size of MoS$_2$ flakes is approximately 0.2–2 μm. Transmission electron microscopy (TEM) was used to investigate the morphology and structure of the sonicated MoS$_2$ nanosheets. The TEM images of MoS$_2$ nanosheets confirm the lattice structure of MoS$_2$ (Figure S1a,b in the Supporting Information). The thinnest of the MoS$_2$ nanosheets obtained were approximately 1.8 nm in thickness (Figure 2b, Figure S2a) while some stacked nanosheets were also evident (Figure S2b). Note, sonication of Li-exfoliated MoS$_2$ had negligible contribution on the oxidation of MoS$_2$, which can be seen from the X-ray photoelectron spectroscopy (XPS) results for the sonicated and original Li-exfoliated MoS$_2$ nanosheets (Figure S3).

To prepare MoS$_2$–MoO$_3$ hybrid nanomaterials, MoS$_2$ nanosheets were first partially oxidized to MoS$_{2-x}$O$_x$ during the spray-coating process in air. The composition of the MoS$_{2-x}$O$_x$ film on a 4H-SiC substrate (referred to as a SiC/MoS$_{2-x}$O$_x$ film; Figure 1b) was confirmed by XPS (Figure 2c). Subsequently, the thermal-annealing-induced crystallization of the MoS$_{2-x}$O$_x$ film was achieved at high temperature, thus forming a SiC/MoS$_{2-x}$O$_x$ film (Figure 1c). The product, namely the MoS$_{2-x}$O$_x$ hybrid nanomaterial, was further characterized by XPS (Figure 2d) and TEM (Figure 2e–g).

The XPS results confirmed the coexistence of Mo$^{4+}$ and Mo$^{6+}$ ions in MoS$_{2-x}$O$_x$ (Figure 2c) and a MoS$_{2-x}$O$_x$ hybrid material obtained after annealing of MoS$_{2-x}$O$_x$ (Figure 2d). The two peaks at 232.6 eV (Mo$^{4+}$ 3d$_{3/2}$) and 229.1 eV (Mo$^{6+}$ 3d$_{3/2}$) in both Figure 2c and Figure 2d are from the semiconducting 2H-phase MoS$_2$, and those at 235.6 eV (Mo$^{6+}$ 3d$_{3/2}$) and 232.2 eV (Mo$^{6+}$ 3d$_{5/2}$) are from MoO$_3$. Note that in Figure 2c, the two peaks located at 231.6 eV (Mo$^{4+}$ 3d$_{3/2}$) and 228.3 eV (Mo$^{4+}$ 3d$_{5/2}$) are assigned to metallic 1T-phase MoS$_2$. The slight decrease detected in the binding energy from 2H-phase to 1T-phase MoS$_2$ was also reported previously.[4b,16] In addition, the coexistence of 1T- and 2H-phase MoS$_2$ is normally found in the lithium-exfoliated MoS$_2$, but the 1T-phase can be completely converted into the stable 2H-phase upon annealing above 300°C.[4b,17] The complete conversion is also confirmed from the XPS result (Figure 2d), where only 2H-phase MoS$_2$ was evident in the MoS$_{2-x}$O$_x$ hybrid material. The coexistence of MoS$_2$ and MoO$_3$ was also confirmed by energy-dispersive X-ray spectroscopy (EDS).
elemental mapping of both MoS$_2$O$_x$ (Figure S4a) and MoS$_2$–MoO$_3$ (Figure S4b). The weight ratio of MoO$_3$ to MoS$_2$ is approximately 2:3, based on the XPS results in Figure 2d.

The low-magnification TEM image of one MoS$_2$–MoO$_3$ fragment is shown in Figure 2e. The selected area electron diffraction (SAED) pattern (Figure 2f) contains signals for both MoS$_2$ and MoO$_3$. We can clearly see (021)-indexed diffraction spots for MoO$_3$ and (100)-indexed diffraction spots for MoS$_2$ in one SAED pattern. This area was further characterized by high-resolution TEM (HRTEM). In Figure 2g, a lattice fringe with a spacing of 0.33 nm was observed, which is consistent with the theoretical lattice spacing of orthorhombic α-MoO$_3$ (021) planes. Meanwhile, the typical MoS$_2$ lattice spacing of 0.27 nm was also observed, which indicates the coexistence of MoS$_2$ and MoO$_3$ in the fragment (Figure 2g).

The X-ray diffraction (XRD) data for experiments based on the MoS$_2$–MoO$_3$ film (Figure S5) also indicated that the annealing process enables the MoS$_2$O$_x$ to crystallize. The crystalline MoS$_2$–MoO$_3$ hybrid nanomaterial was confirmed to be formed based on the TEM results (Figure 2e–g). The formation of the nanomaterial was further verified from the XRD patterns, in which a strong (021) peak attributable to crystalline MoS$_2$–MoO$_3$ (021) planes and (100)-indexed diffraction spots for MoO$_3$ and (100)-indexed diffraction spots for MoS$_2$ in one SAED pattern. This area was further characterized by high-resolution TEM (HRTEM). In Figure 2g, a lattice fringe with a spacing of 0.33 nm was observed, which is consistent with the theoretical lattice spacing of orthorhombic α-MoO$_3$ (021) planes. Meanwhile, the typical MoS$_2$ lattice spacing of 0.27 nm was also observed, which indicates the coexistence of MoS$_2$ and MoO$_3$ in the fragment (Figure 2g).

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A Hall measurement was performed to characterize the doping characteristics of the MoS$_2$–MoO$_3$ hybrid film. The film has p-type hole conductivity with a measured doping concentration of 10$^{16}$–10$^{18}$ cm$^{-3}$. As a proof-of-concept application, the light-emitting diode (LED) device, with an n-SiC/p-MoS$_2$–MoO$_3$ heterojunction as the active layer, was fabricated (see detailed device structure and fabrication in Figure 1d, and Experimental Section). The SEM crosssection image in Figure S6 reveals that the thickness of the prepared MoS$_2$–MoO$_3$ film is approximately 3 μm.

Figure 3a shows the current-voltage (I-V) curve measured for the prepared LEDs (device structure given in Figure 1d). It can be seen that the LED device exhibits a turn-on voltage of approximately 4.5 V. When the applied forward bias was increased to 10 V, the current reached approximately 15 mA. The inset in Figure 3a shows a lighting photo of the LED device taken at forward bias of 18 V, where we can see the intense light emission from the transparent ITO electrode (ITO = indium tin oxide) of the LED. In combination, the I-V characteristics and light emission of the n-SiC/p-MoS$_2$–MoO$_3$ heterojunction LED device indicate that the MoS$_2$–MoO$_3$ hybrid nanomaterial works efficiently as a p-type hole-injection layer in the device. Figure 3b shows the EL spectra of the LED device biased at different forward voltages. The EL spectra show broad emission profiles with four sub-bands located at λ = 411, 459, 553, and 647 nm, respectively, after fitting the spectrum taken at 18 V (inset in Figure 3b).

To understand the origins of the peaks detected in the EL spectrum and the p-type hole conductivity associated with defects in the MoS$_2$–MoO$_3$ layer, first-principle calculations were performed to investigate the electronic properties and the alignment of energy levels in MoS$_2$–MoO$_3$. First, the effect of point defects in MoS$_2$ was neglected, since the sulfur vacancy, which is one of the most likely defect types in a MoS$_2$ film, has shown to create deep gap states and is unlikely to give rise to the measured p-type conductivity. Second, the possibility of oxygen substitution of sulfur in MoS$_2$ is ruled out because there is no defective state in the band gap resulting from the substitution (Figure S7).

We are particularly interested in the defects in MoO$_3$, which are probably introduced during the oxidation of MoS$_2$ to form MoO$_3$. The proposed oxygen-deficient oxide components consist of several intermediate molybdenum oxides, such as MoO$_3^-$ or MoO$_4^-$, which accompany the deep defective state, that is, the oxygen vacancy (V$_O$), about 1 eV below the CB localized on the neighboring Mo atoms (labeled as D1, Figure 4e).[21] On the other hand, the incomplete oxidation of MoS$_2$ during thermal treatment is highly possible. As a result, sulfur atoms from MoS$_2$ can occupy the site for oxygen atoms in MoO$_3$. These defects may be considered as an S substitution of an O atom (denoted as $S_O$) in the MoO$_3$. The α-MoO$_3$ phase involves three types of oxygen atoms, that is, the singly coordinated oxygen (O1), twofold-coordinated oxygen (O2), and threefold-coordinated oxygen atom (O3). Sulfur substitutions of O1, O2, and O3 atoms are labeled as $S_{O1}$, $S_{O2}$, and $S_{O3}$, respectively (Figure 4a). In contrast to the V$_O$ defect, plots of density of states (DOS) in Figure 4a show that these $S_O$ defects create defective states which are overlapped and located about 0.5 eV above the VB (labeled as D2, Figure 4e). The D2 states of $S_{O1}$, $S_{O2}$, and $S_{O3}$ defects are found to have p$_x$(S)-d$_x$(Mo), p$_y$(S)-d$_y$(Mo), and p$_z$(S)-d$_y$(Mo) hybridization, with a p:d orbital occupation ratio of 1:0.40, 1:0.41, and 1:0.29, respectively. These defective states above the VB of MoO$_3$ play an important role in both producing the p-type carriers and giving rise to the features observed in the
Transition 2 corresponds to the transition from the CB of MoO$_3$ to the VO-related D$_1$ level to the VB of MoO$_3$. The work function of Au/Ti can partially relax nonradiatively to separate for clarity. Under the forward bias, the injected electrons from the CB of the SiC substrate can relax to the CBs of MoO$_3$, and holes can be directly injected onto the VBs of MoO$_3$. This occurs as the injected electrons from the CB of the SiC substrate can relax to the CBs of MoO$_3$, and holes can be directly injected onto the VBs of MoO$_3$. The peak at $\lambda = 647$ nm (1.92 eV), that is, the fourth emission, arises from the recombination of electrons and holes in the MoO$_3$ layer. Owing to the applied voltage and weak screening effect in the atomically thin MoS$_2$ layer, its Fermi level can shift below the valence-band maximum. Therefore, the injected holes from ITO to MoS$_2$ can accumulate at the top valence band at the K point of the Brillouin zone, which relates to recombination of the A exciton with peak positions which are nearly insensitive to thickness (approximately 1.86–1.89 eV). With this in mind, we used single-layer MoS$_2$, in the theoretical calculations for simplicity, as illustrated in Figure 4e. The other two peaks, that is, at $\lambda = 459$ nm (2.7 eV) and $\lambda = 553$ nm (2.24 eV), are related to the radiative recombination of carriers occupying D1 and D2 defective levels in the MoO$_3$ layer. The emission at $\lambda = 459$ nm arises from the recombination of electrons at the CB with holes at the D2 level in MoO$_3$, whereas the emission centered at $\lambda = 553$ nm is likely to arise from the transition from the V$_O$-related D1 level to the VB of MoO$_3$. As a result of the lattice distortion and defects in the layers, these emission bands are broadened. The experimental data are consistent with the theoretically predicted emission bands from the LED devices (Table 1).

![Figure 4](image.png)

**Figure 4.** a) DOS of spin-up (black lines) and spin-down (gray lines) electrons in MoO$_3$ containing S$_{SO1}$, S$_{SO2}$, and S$_{SO3}$ defects. The arrows indicate the defective states in the band gap. b–d) Isosurface plots of the charge density of the defective states of S$_{SO1}$ (b), S$_{SO2}$ (c), and S$_{SO3}$ (d). e) Energy diagram for the hybrid systems composed of 4H-SiC, MoS$_2$, and MoO$_3$. Electroluminescence transition scheme is plotted. Transition 1 corresponds to the transition from the CB to the VB of MoO$_3$. Transition 4 corresponds to the recombination of electrons at the CB and holes at the top valence band at the K point of the Brillouin zone of MoS$_2$, with thickness from a single layer to a few layers. Single layer MoS$_2$ was used in (e) to illustrate the band gap, where the dashed lines within the band gap represent the slight decrease of the gap with increasing the number of layers of MoS$_2$. Transition 2 corresponds to the transition from the CB of MoO$_3$ to the S$_{SO2}$-related (x = 1, 2, 3) D$_2$ level, whereas transition 3 is from the V$_O$-related D1 level to the VB of MoO$_3$. The work function of Au/Ti (4.75 eV) and ITO (4.7 eV) is taken from Refs. [31a,b]. The electron affinity for 4H-SiC (3.1 eV), MoS$_2$ (4.2 eV), and MoO$_3$ (2.3 eV) was obtained from Refs. [31c,d,e].

**Table 1:** Experimental and theoretical EL transitions for n-SiC/p-MoS$_2$–MoO$_3$ hybrid nanomaterials and deserves further detailed exploration.

<table>
<thead>
<tr>
<th>Transition</th>
<th>EL peaks (experimental)</th>
<th>EL peaks (theory)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CB (MoO$_3$)</td>
<td>$\lambda = 411$ nm (3.02 eV)</td>
<td>$\lambda = 400$ nm (3.1 eV)</td>
</tr>
<tr>
<td>→VB (MoO$_3$)</td>
<td>$\lambda = 459$ nm (2.7 eV)</td>
<td>$\lambda = 459$ nm (2.7 eV)</td>
</tr>
<tr>
<td>CB (MoS$_2$)</td>
<td>$\lambda = 553$ nm (2.24 eV)</td>
<td>$\lambda = 590$ nm (2.1 eV)</td>
</tr>
<tr>
<td>→D1</td>
<td>$\lambda = 647$ nm (1.92 eV)</td>
<td>$\lambda = 653$ nm (1.9 eV)</td>
</tr>
<tr>
<td>CB (MoS$_2$)</td>
<td>$\lambda = 647$ nm (1.92 eV)</td>
<td>$\lambda = 653$ nm (1.9 eV)</td>
</tr>
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Previous studies of MoS$_2$ have demonstrated the important and effective role of appropriate contacts in tuning the Schottky barriers. The addition of a thin oxide barrier, such as MgO [29] and TiO$_2$ [30], can greatly eliminate the contact resistance and alleviate the conduction mismatch. The ability to tune the height and width of the Schottky barrier by contact engineering opens the possibility to tune the mobility and polarity of conducting carriers. Similarly, the Schottky barrier formed between the MoS$_2$–MoO$_3$ hybrid film and the metal contacts tends to be not only determined by the work function, but also affected by the significant interfacial states and defective states. Controlling the Schottky barriers will be very important in potential devices based on MoS$_2$–MoO$_3$ hybrid nanomaterials and deserves further detailed exploration.
In conclusion, a facile preparation strategy for MoS$_2$–MoO$_3$ hybrid nanomaterials was developed through heat-assisted partial oxidation of MoS$_2$ nanosheets in air followed by the subsequent thermal-annealing-driven crystallization. The obtained MoS$_2$–MoO$_3$ material exhibited p-type conductivity. As a proof-of-concept application, a n-SiC/p-MoS$_2$–MoO$_3$ heterojunction was applied in LEDs. The origins of EL peaks from these devices were theoretically explored and it was shown that radiative recombination processes relating to band edges and defect energy levels played key roles. We believe that our facile synthesis of hybrid nanomaterials for functional applications may provide opportunities to develop new advanced 2D hybrid nanomaterials for various applications in optoelectronics, clean energy, and information storage.

**Experimental Section**

**Preparation of MoS$_2$–MoO$_3$ hybrid nanomaterials: Molybdenum disulfide (MoS$_2$, of size 10–30 μm) was purchased from Rose Mill (West Hartford, USA). The detailed electrochemical lithium-intercalation method for preparation of MoS$_2$ nanosheets was described in our previous report.**

Herein, after the lithium-intercalated MoS$_2$ nanosheets were sonicated in a water bath for 3 h, they were washed with Milli-Q water twice by centrifugation and redispersed in water. The sonicated MoS$_2$ nanosheets were deposited on a solid substrate, such as Si, SiC, quartz, or glass, by the spray-coating method. The MoS$_2$ suspension was then carefully sprayed onto the SiC substrate. After the coating process, the substrate was heated on a hot plate at 90°C to accelerate the solvent evaporation and increase the oxidation content of MoS$_2$. Subsequently, the obtained MoS$_2$–O was annealed in 5% H$_2$–Ar gas at 450–500°C for 1 h to crystallize the MoS$_2$–MoO$_3$ hybrid nanomaterials. The detailed film preparation and annealing experiments are presented in the device fabrication section (see below), where the SiC substrate was used.

**Characterization:** Scanning electron microscopy (SEM) was performed using a JEOL JSM-7600F field-emission scanning electron microscope analyzer at an accelerating voltage of 5 kV. Elemental distribution mapping based on energy-dispersive X-ray spectroscopy was determined with a JEOL JSM-7600F field-emission scanning electron microscope analyzer under transmission mode using the transmission electron detector (TED). Atomic force microscopy (AFM) images and thickness measurements were obtained using tapping-mode AFM (Dimension ICON with Nanoscope V controller, Bruker). X-ray photoelectron spectroscopy characterization (XPS, Axis Ultra) was utilized to characterize elemental composition. Transmission electron microscopy (TEM), high-resolution TEM (HRTEM), and selected area electron diffraction (SAED) were performed on a JEOL 2100F with a beam energy of 200 keV. X-ray (HRTEM), and selected area electron diffraction (SAED) were performed using a JEOL JSM-7600F field-emission scanning electron microscope (dimension JSM-7600F with Nanoscope V controller, Bruker) as the spray-coating method with the Peredw-Burke-Erzerhof functional (PAW-PBE) were performed. A cutoff energy of 400 eV and 2 /C148 2 /C148 mesh in k-space were adopted. A 3 × 3 × 3 supercell was used and the structures were relaxed until the Hellmann-Feynman forces become less than 0.01 eV Å$^{-1}$. Since the lack of self-interaction corrections in normal DFT fails to reproduce electronic features of the highly delocalized defective states in d oxides such as TiO$_2$ and MoO$_3$, the hybrid functionals (HSE06) were used to calculate the defective states in the band gap. The calculated band gap of MoO$_3$ is 3.10 eV which is consistent with the experimental value of approximately 3.2 eV.

Theoretical calculation: The calculation was performed using the planewave code Vienna ab initio simulation package (VASP). Spin-polarized calculations using the projector augmented wave method with the Perdew-Burke-Ernzerhof functional (PAW-PBE) were performed. A cutoff energy of 400 eV and 2 /C148 2 /C148 mesh in k-space were adopted. A 3 × 3 × 3 supercell was used and the structures were relaxed until the Hellmann-Feynman forces become less than 0.01 eV Å$^{-1}$. Since the lack of self-interaction corrections in normal DFT fails to reproduce electronic features of the highly delocalized defective states in d oxides such as TiO$_2$ and MoO$_3$, the hybrid functionals (HSE06) were used to calculate the defective states in the band gap. The calculated band gap of MoO$_3$ is 3.10 eV which is consistent with the experimental value of approximately 3.2 eV.

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