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Progress in the Application of Mo_xC-based Materials for Electrolysis of Water

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Abstract

Driven by the dual-carbon goal, hydrogen energy, which has the advantages of cleanliness, non-pollution, long-term storage and high energy density, would act a significant impact in the development process of energy transition. Electrocatalytic hydrolysis was one of the most outstanding and cleanest strategies for large-scale hydrogen preparation. Molybdenum carbide showed enormous potential in the field of electrocatalytic hydrolysis due to its unique electronic structure features. In this paper, the synthetic carriers of Mo_xC-based water decomposition electrocatalysts were reviewed, and their four nanomorphology modification strategies were summarized: zero-dimensional spatial angle, one-dimensional spatial angle, two-dimensional spatial angle, and three-dimensional spatial angle. Finally, the obstacles and prospects for the further development of Mo_xC-based catalysts were discussed to supply some reference value for the advancement of this field.

Keywords

Molybdenum Carbide; Morphology; Hydrolysis; Electrocatalysts; Synthetic Carriers.

1. Introduction

Currently, in research on overall electrocatalytic water splitting (OWS), noble metal-based electrode catalyst materials such as Pt, Pd, Ru and Ir are more efficient, but the high cost restricted their practical usage[1, 2]. Thus, the study of high-performance and inexpensive electrode catalysts has become an inevitable choice. Transition metal-based composites have been extensively investigated in electrocatalytic studies due to the adjustable d orbitals[3, 4]. Among the many transition metals, molybdenum-based electrocatalysts are particularly useful, on the one hand, molybdenum has high reserves on earth and its price was much lower than the commonly used Ni metal; on the other hand, molybdenum-based materials had unique electronic structure and nanostructure [5-7].

Molybdenum-based catalysts that were commonly used for electrocatalytic water splitting included Mo_xC[8], MoN_x[9], MoS_2[10], $MoSe_2$[11], and MoO_x[12]. Among them, Mo_xC demonstrated excellent corrosion resistance, electrical conductivity, and stability, which had attracted increasing attention in the field of energy conversion. Notably, Mo_xC exhibited the characteristics of hydrogen adsorption (ΔG_{H^*}) similar to that of Pt, enabling high activity across a broad pH range[13]. Kitchin et al.[14] conducted DFT calculations on Mo_xC and found that the introduction of C into the carbide surface induced lattice tensile strain. Contrasted with single-metal surfaces, the carbide-metal surface exhibited stronger hydrogen adsorption. Additionally, the value of ΔG_{H^*} was closely associated with the d-band center of the molybdenum carbide surface, resembling the adsorption behavior of noble metal Pt in water electrolysis. Studies had shown that the adsorption and activation of reactant molecules by the catalyst were crucial for catalytic performance. Given its surface adsorption behavior and electronic structure characteristics similar to those of platinum, Mo_xC played a significant role in electrocatalytic water splitting.

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However, Mo_xC exhibited poor electrical conductivity for water-splitting catalysis. Introducing a conductive substrate during its preparation had been considered a feasible strategy to optimize electron transport. Moreover, due to nanoparticle agglomeration and limited specific surface area, the active sites of Mo_xC-based materials were insufficiently exposed. To address this issue, researchers had employed synthetic supports to enhance catalyst dispersion and regulate its nanostructure, thereby optimizing catalytic activity.

Based on existing research, this study summarized the synthetic supports for Mo_xC-based electrocatalysts for OWS and outlined the nanostructure regulation strategies from the perspectives of 0 D, 1 D, 2 D, and 3 D structures.

2. Synthetic Supports for Mo_xC-Based Electrocatalysts

2.1 Carbon-Based Materials

Carbon-based materials, due to their high charge-transfer efficiency, expansive surface area, and durable stability, were widely used in the construction of Mo_xC-based electrocatalysts for water splitting. Common types included graphene, carbon nanotubes, porous carbon, and carbon fibers.

Lin et al.[15]used graphene as a support to synthesize the Mo_2C-Ru@RGO composite materials (**Figure 1.a**). In 1 M KOH, Mo_2C-Ru@RGO exhibited excellent HER performance, surpassing the commercial Pt/C electrode by 20% in electrochemical performance. DFT results indicated that the synergistic effect of dual electroactive species effectively reduced the metal-hydrogen bonding strength. Furthermore, interface reconstruction between Mo_2C-Ru and graphene improved the efficiency of electron transfer. Das et al.[16]developed a Ni/MoxC-NC catalyst using a simple synthesis strategy, where graphene-carbon nanotubes (NC) served as the support material (**Figure 1.b**). This catalyst demonstrated outstanding the activity of OWS in 1 M KOH. DFT calculations confirmed the existence of an electronic synergistic interaction among Mo_xC, Ni, and NC, with electron transfer occurring in the direction of Ni → MoxC → NC. Lv et al.[17]synthesized a novel self-supporting multichannel electrocatalyst through electrospinning-carbonization technology (**Figure 1.c**). The prepared [MoC/C]//[Ni/C]-NMCFs catalyst exhibited excellent stability in both HER and OER processes. Moreover, the synergistic interaction between MoC and Ni enhanced the efficiency of electrocatalytic water splitting. Hui et al.[18]employed a molten salt strategy to prepare ultrafine Mo_2C nanoparticles using biomass-derived guar gum porous carbon nanosheets as the support (**Figure 1.d**). The high viscosity of guar gum provided a spatial confinement effect, mitigating nanoparticle aggregation.

A comparison of the electrochemical performance of Mo_xC-based materials using carbon-based supports is presented in **Table 1**.

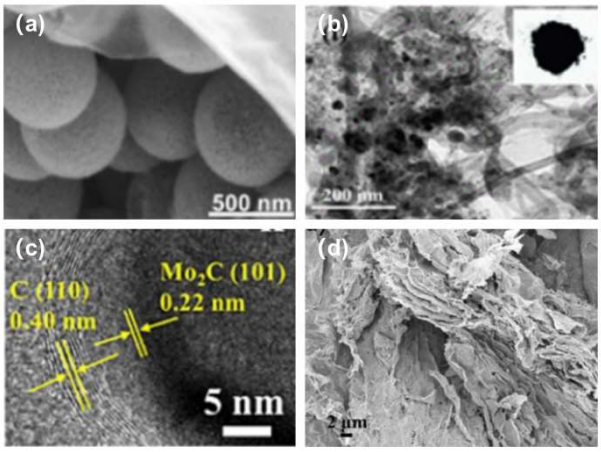

Figure 1. (a) SEM image of Mo_2C-Ru@RGO[15], (b) TEM image of Ni/Mo_xC-NC[16], (c) HRTEM image of [MoC/C]//[Ni/C]-NMCFs[17] (d) SEM image of Mo_2C/NCS[18].

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Table 1. Four samples comparing

Catalysts	Electrolyte	HERη_{10} / (mV)	OERη_{10} / (mV)	References
Mo_2C-Ru@RGO	1 M KOH	62	324	[15]
Ni/Mo_xC-NC	1 M KOH	43	~	[16]
[MoC/C]//[Ni/C]-NMCFs	1 M KOH	161	328	[17]
Mo_2C/NCS	0.5 M H_2SO_4	125	~	[18]

2.2 Nickel Foam

Nickel foam (NF), as one of the most widely used conductive supports, has been applied in the construction of three-dimensional, self-supported Mo_xC electrocatalysts. He et al.[19]employed a hydrothermal-calcination method employing glucose as the carbon source to fabricate a Mo_2C@NF-850 electrocatalyst, as displayed from **Fig. 2.a-b**. The carbon layer originating from glucose improved the dispersion of the catalyst and also protected Mo_2C from corrosion by the electrolyte, thereby enhancing its stability during electrocatalysis. Additionally, in alkaline electrolyte, the catalyst exhibited excellent HER activity. Lei et al.[20]developed a simple strategy using NF as the synthesis support to anchor MoS_2 quantum dots (QDs) on the surface of molybdenum carbide, creating an atomic-level heterojunction, as visualized in **Fig. 2.c-d**. Theoretical computation confirmed that the Mo surface of Mo_2C acted as an electron trap, which accelerated the vertical charge migration from MoS_2 QDs to Mo_2C and enriched the electrons on the Mo surface. The obtained MoS_2 QDs@Mo_2C@NF exhibited exceptional catalytic activity for OER. Xu et al.[21]fabricated a Ni-Mo_2C/NC Mott-Schottky array using NF as the support via a self-assembly-carbothermal strategy, as shown in **Fig. 2.e-f**. This catalyst served as a bifunctional electrocatalyst and exhibited superior electrochemical performance compared to Pt/C||RuO_2. DFT calculations indicated that the incorporation of nickel and N-doped carrier altered the electronic structure of Mo_2C, resulted in enhancing its catalytic activity.

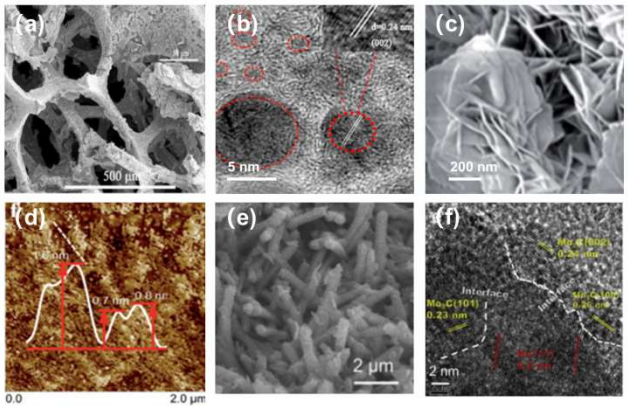

Figure 2. (a-b) SEM and TEM images of Mo_2C@NF-850[19], (c-d) FE-SEM and AFM images of MoS_2 QDs@Mo_2C@NF[20], (e-f) SEM and HRTEM images of Ni-Mo_2C/NC[21].

Table 2. Three samples comparing

Catalysts	Electrolyte	HERη_{10} / (mV)	OERη_{10} / (mV)	References
Mo_2C@NF-850	1 M KOH	42	~	[19]
MoS_2 QDs@Mo_2C@NF	1 M KOH	~	190	[20]
Ni-Mo_2C/NC	1 M KOH	45	337	[21]

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Table 2 provided a comparison of the HER and OER activity of Mo_xC-based materials supported on nickel foam.

2.3 Other Synthesis Supports

Metal-organic frameworks (MOFs), MXene ($Ti_3C_2T_x$), and TiO_2 have also been additionally employed as supports for the construction of Mo_xC electrocatalysts. Ali et al.[22]prepared Mo_2C/UiO-66 catalysts using a zirconium-based MOF (UiO-66) as the synthesis support via a solvothermal method, which exhibited excellent overall electrocatalytic water splitting performance. Tang et al.[23]used a two-dimensional mesoporous MXene nanosheet as the support to fabricate mNC-MoC/Ti_3C_2 catalysts, which demonstrated excellent water splitting activity in acidic media. Shi et al.[24]used TiO_2 as a support to prepare Mo_2C@TiO_2 electrocatalysts, which exhibited superior HER activity.

3. Morphology Regulation Strategies

Generally, the specific surface area of electrocatalytic materials largely influenced their catalytic performance, and the specific surface area was directly related to the microscopic morphological structure. Therefore, researchers have investigated molybdenum carbide with different microscopic morphological structures, including 0D nanoparticles, 1D nanorods/nanowires/nanotubes, 2D nanosheets, and 3D composite structures.

3.1 0 D (Ero-Dimensional) Structure of Mo_xC

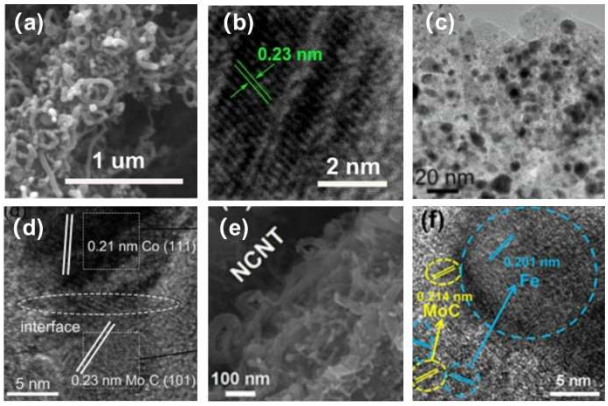

Figure 3. (a-b) SEM and HR-TEM images of Co/Mo_2C-NCNTs[25], (c-d) TEM and HRTEM images of Co/Mo_2C@C[26], (e-f) FE-SEM and HRTEM images of MoC-Fe@NCNT[27].

Table 3. Three samples comparing

Catalysts	Electrolyte	HERη_{10} / (mV)	OERη_{10} / (mV)	References
Co/Mo_2C-NCNTs	1 M KOH	98	254	[25]
Co/Mo_2C@C	1 M KOH	170	310	[26]
MoC-Fe@NCNT	1 M KOH	50	304	[27]

0 D nanomaterials could enhance the value of BET by reducing the size of molybdenum carbide (Mo_2C) nanoparticles and increasing the porosity. This also benefited from using a high surface area substrate to improve the dispersion of nanoparticles, thus enhancing the materials HER catalytic activity. Zhang et al.[25]employed a simple electrospinning method to prepare bifunctional Co/Mo_2C nanoparticles (Co/Mo_2C-NCNTs) grown on 3 D layered N-doped carbon nanotubes (NCNTs), as shown in **Figure 3.a-b**. The marked cooperative effect between Co and Mo_2C nanoparticles optimized the adsorption strength of catalyst on reaction intermediates, thus enhancing the HER and OER performance. Electrochemical data indicated that Co/Mo_2C-NCNTs exhibited excellent stability

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during HER and OER processes. Yuan et al.[26] synthesized Co/Mo_2C@C catalysts using a simple phase separation method, as demonstrated in **Figure 3.c-d**. BET analysis revealed that Co/Mo_2C nanoparticles exhibited microporous characteristics, which enhanced the contact area between the Co/Mo_2C and electrolyte during the catalytic reaction. DFT calculations showed that cobalt could enhance Mo_2C HER activity through electronic synergistic effects. After OER, Co was oxidized to CoOOH, which further contributed to enhancing OER activity. Huang et al.[27]used a self-assembly-pyrolysis strategy to prepare MoC-Fe nanoparticles grown on porous nitrogen-doped carbon nanotubes (NCNTs), as shown in **Figure 3.e-f**. The synthesized MoC-Fe@NCNT exhibited excellent HER and OER activity. DFT calculations confirmed that NCNTs acted as electron communication amplifiers, facilitating electron transfer and inhibiting the aggregation and corrosion of active species. Additionally, the heterojunction between MoC-Fe exhibited synergistic effects, imparting excellent bifunctional electrocatalytic performance. The electrochemical performance comparison of 0D Mo_xC-based materials was shown in **Table 3**.

3.2 1 D (One-Dimensional) Structure of Mo_xC

Zhang et al.[28]employed a heat-treatment-coating-hydrothermal strategy to prepare a Mo_2C@g-C_3N_4@NiMn-LDH bifunctional catalyst, using Mo_2C nanowires as the growth template, as shown in Figure 4a-b. From the morphological structure, Mo_2C and NiMn-LDH were positioned on the inner and outer walls of g-C_3N_4, respectively. In the composite material, Mo_2C@g-C_3N_4 served as the main catalytic center for HER, while the external NiMn-LDH played as a cocatalyst. For OER, the active site was primarily the g-C_3N_4@NiMn-LDH, with Mo_2C acting as a cocatalyst. Al Mahmud et al.[29]designed a electrocatalyst, integrated molybdenum carbide (MoC), nickel carbide (NiC), and nitrogen-doped reduced graphene oxide (N-rGO) in a single heterostructure, using a hydrothermal-calcination strategy. SEM and TEM results revealed that MoC/NiC exhibited a nanorod structure, which was uniformly dispersed on the layered N-rGO, as shown in Figure 4c-d. Electrochemical tests demonstrated that the MoC/NiC@N-rGO composite exhibited excellent HER and OER activity. The dual-electrode system composed of this catalyst displayed outstanding stability during overall electrocatalytic water splitting. Li et al.[30]used MoO_3 nanowires as a template and employed a polydopamine organic layer for carbon infiltration, preparing Mo_2C nanotubes (Mo_2C NTs) with an ultra-thin tiled structure. Nitrogen doping was then introduced into the nanotubes via chemical vapor deposition, successfully synthesizing an N-Mo_xC catalyst, as shown in Figure 4e-f. Electrochemical tests indicated that N-Mo_xC exhibited excellent alkaline HER activity. A comparison of the electrochemical performance of 1D (one-dimensional) Mo_xC-based materials is shown in Table 4.

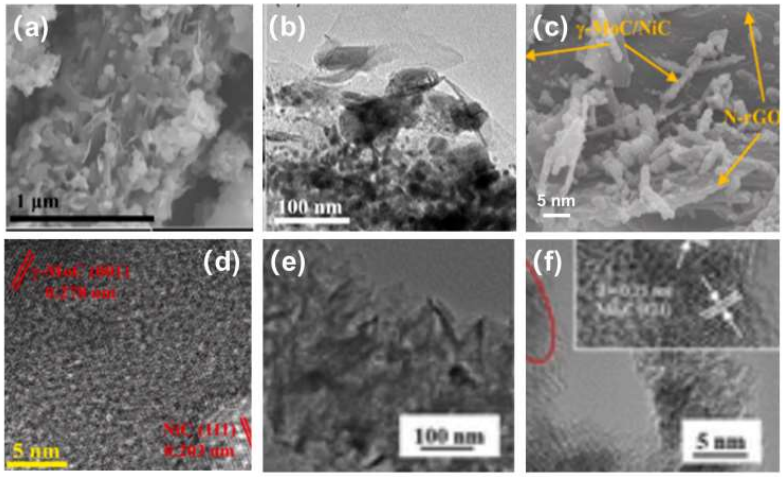

Figure 4. (a-b) SEM and TEM images of Mo_2C@g-C_3N_4@NiMn-LDH[28], (c-d) TEM and HRTEM images of MoC/NiC@N-rGO[29], (e-f) SEM and HRTEM images of N-Mo_xC[30].

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Table 4. Three samples comparing

Catalysts	Electrolyte	HERη_{10} / (mV)	OERη_{10} / (mV)	References
Mo_2C@g-C_3N_4@NiMn-LDH	1 M KOH	116	290	[28]
MoC/NiC@N-rGO	0.5 M H_2SO_4	185	298	[29]
N-Mo_xC	1 M KOH	120	~	[30]

3.3 2 D (Two-Dimensional) Structure of Mo_xC

Gu et al.[31]prepared nitrogen-doped Mo_2C nanosheets using a metal-organic framework (MOF) as carrier, whose morphological features were shown in **Figure 5.a-b**. The synthesized Mo_2C/Co@NC catalyst shown outstanding electrocatalytic performance during HER, OER, and oxygen reduction reaction (ORR). An interface coupling effect between Mo_2C and the Co@NC support was observed, which facilitated the optimization of the electronic structure, thus resulted in the enhanced catalytic performance. Liu et al. [32]developed a feasible process by hydrothermally preparing $NiMoO_4$ nanosheets on CC, followed by chemical vapor deposition (CVD) and calcination, during which active metal species formed on the $NiMoO_4$ precursor and catalytically grew carbon nanotube (CNT) arrays on the outer side of the nanosheets, shown in **Figure 5.c-d**. The prepared CNT/MoC/NMC-3 nanocomposite retained its two-dimensional structure. Electrochemical analysis demonstrated that the electrode exhibited excellent HER and OER performance. DFT calculations confirmed that, at negative potentials, MoC and CoNiMo alloys were induced, with active HER sites formed on the molybdenum surface. Additionally, the parallelly aligned nanosheets and the CNT arrays, extending outward from the plane, accelerated gas detachment and increased the contact surface area with the electrolyte. Diao et al.[33]employed a heteroatom modification strategy to prepare arrayed, nitrogen-doped molybdenum carbide nanosheets, as shown in **Figure 5.e-f**. X-ray absorption fine structure characterization confirmed the electronic modulation of Mo_2C by nitrogen. Electrochemical tests indicated that the synthesized N-Mo_2C/NF exhibited excellent HER and OER catalytic activity. DFT calculations confirmed that doping with highly electronegative nitrogen significantly optimized the electronic structure of Mo_2C, thereby improving the adsorption/desorption of active species during the HER/OER processes. A comparison of the electrocatalytic capability of 2D Mo_xC-based materials was shown in **Table 5**.

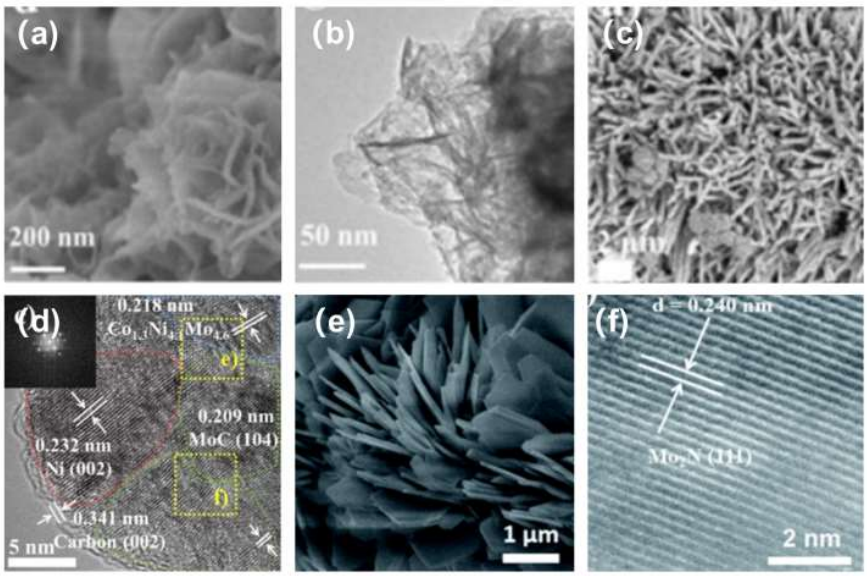

Figure 5. (a-b) SEM and TEM images of Mo_2C/Co@NC[31], (c-d) SEM and HRTEM images of CNT/MoC/NMC-3[32], (e-f) SEM and HRTEM images of N-Mo_2C/NF[33].

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Table 5. Three samples comparing

Catalysts	Electrolyte	HERη_{10} / (mV)	OERη_{10} / (mV)	References
Mo_2C/Co@NC	1 M KOH	51	308	[31]
CNT/MoC/NMC-3	1 M KOH	51	226	[32]
N-Mo_2C/NF	1 M KOH	83.9	220	[33]

3.4 3 D (Three-Dimensional) Structure of Mo_xC

Molybdenum carbide in 3D structure possessed a layered or interconnected framework, which imparted excellent mechanical stability to the material. It also offered a large surface area, favoring the exposure of electroactive sites. Meng et al.[34]prepared a novel 3 D hierarchical macro-meso-microporous Mo_2C (3DHP-Mo_2C) via a simple and scalable salt-template way, which was shown in Figure **6.a-b**. The 3DHP-Mo_2C structure, with its clear and hierarchical macro, meso, and micropores, significantly enhanced mass and electron transfer, while also considerably increasing the specific surface area, promoting greater exposure of active sites, which improved the catalytic performance in 0.5 M H_2SO_4 and 1 M KOH for HER. Peng et al.[35]demonstrated an in-situ synthesis strategy to synthesize a 3D flower-like heterojunction FeNi-Mo_2C/CF catalyst. **Figure 6.c-d** displayed the 3 D morphological features. The resulting catalyst exhibited efficient performance of water electrolysis. Furthermore, the overall water-splitting device composed of FeNi-Mo_2C/CF demonstrated stable operation performance. Hou et al.[36]prepared a 3 D Mo_2C nanosphere, with the doping of Ni single atom, using a hydrothermal-pyrolysis strategy, as shown in Figure 6e-f. Nickel atoms were doped into Mo_2C in the form of Ni-O-Mo bridge bonds. In-situ synchrotron XAS revealed that after HER, both the coordinating number and bond length of the Ni-O-Mo bond changed, but the nickel species remained in an atomic dispersed state; after OER, the atomically dispersed Ni aggregated into very small clusters, and new Ni-O-Ni bond was formed. DFT analysis confirmed that the configuration of single-atom nickel is crucial for optimizing both HER and OER activity. A comparison of the performanc of electrolysis of water of 3D Mo_xC-based materials was shown in **Table 6**.

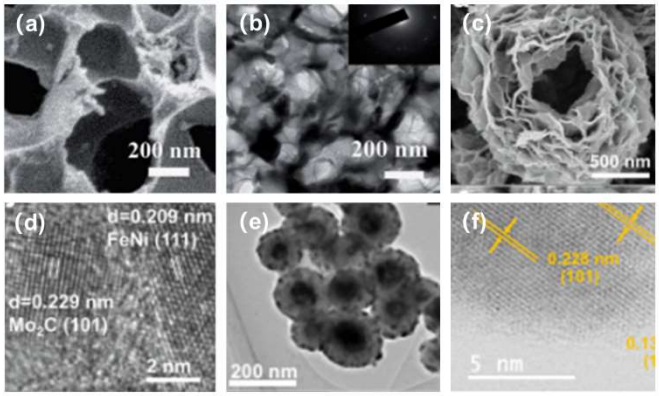

Figure 6. (a-b) SEM and TEM images of 3DHP-Mo_2C[34], (c-d) SEM and HRTEM images of FeNi-Mo_2C/CF[35], (e-f) SEM and HRTEM images of NiSA-O/Mo_2C[36].

Table 6. Three samples comparing

Catalysts	Electrolyte	HERη_{10} / (mV)	OERη_{10} / (mV)	References
3DHP-Mo_2C	1 M KOH	139	~	[34]
FeNi-Mo_2C/CF	1 M KOH	81	228	[35]
Ni_{SA}-O/Mo_2C	1 M KOH	133	299	[36]

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4. Conclusion and Outlook

Molybdenum carbide (Mo_xC), due to its unique electronic structure and excellent conductivity, shown great potential in the field of electrocatalysis. This paper summarized the synthesis carriers for Mo_xC, and discussed in detail four morphological modification strategies for Mo_xC-based electrocatalysts, providing a deeper understanding for optimizing electrocatalytic performance. Although the advantages of molybdenum carbide-based catalysts in electrocatalytic water splitting were well-known, their practical applications still faced significant challenges.

To further explore the catalytic mechanisms, it is necessary to combine DFT calculations and in situ characterization techniques to explain the possible structure-activity relationships, thereby providing guidance for the design and optimization of Mo_xC composite materials with high electrocatalytic water splitting activity. It remains essential to develop novel synthesis strategies to facilitate the regulation of catalyst composition and structure. Therefore, developing simple synthesis methods to fabricate highly active and stable molybdenum carbide catalysts is highly attractive.

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