

Electronic Supplementary Material

Emerging noble metal-free Mo-based bifunctional catalysts for electrochemical energy conversion

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Table S1 Overall water splitting performance of Mo-based catalysts in 1.0 M KOH (except for special noting)
Voltage (V) values are calculated with respect to reversible hydrogen electrode (RHE) unless specified
§ denotes HER/OER/ORR trifunctional catalysts

HER/OER Catalyst	Full cell voltage (V) @10 mA cm ⁻² except for special noting	Cell stability test (h)	Ref.
Mo chalcogenides			
Fe-Doped MoS ₂ Nanocanopies on Ni foam (Fe:MoS ₂)	1.52	140	[43]
Co doped MoS ₂ nanosheets (Co:MoS ₂)	1.58	~13.89	[135]
Co and Nb doped MoS ₂ nanosheets shelled micro-TiO ₂ hollow spheres §	1.57	60	[353]
Hierarchical nanoassembly of MoS ₂ /Co ₉ S ₈ /Ni ₃ S ₂ /Ni foam	1.54	20	[3]
Distorted inverse spinel Ni–Co–O layer on the MoS ₂ plate grown on C paper (NiCo ₂ O ₄ @MoS ₂)	1.72	2	[146]
Coupled MoS ₂ /FeOOH shelled Ni ₃ S ₂ nanowires grown on Ni foam (Ni ₃ S ₂ @MoS ₂ /FeOOH)	1.57	50	[46]
MoS ₂ nanosheets and Ni ₂ P nanoparticles shelled MoO ₂ sub-micron wires grown on Ti foil	1.72	10	[44]
MoS ₂ nanosheets grafted porous Co particles embedded in N doped C flakes grown on C nanofibers (CoNC@MoS ₂)	1.62	~55.55	[149]
Bimetallic CoNi-zeolitic imidazole framework embedded by MoS ₂ nanosheets (MoS ₂ @CoNi-ZIF)	1.55	40	[147]
C layer coated Ni ₃ S ₂ /MoS ₂ nanohybrids	1.76	15	[145]
NiCo ₂ S ₄ nanostructure coated by MoS ₂ nanosheets grown on Ni foam (MoS ₂ /NiCo ₂ S ₄)	1.49	40	[148]
MoS ₂ and CoP heterostructure loaded on N, P-doped C §	1.67	24	[354]
MoS ₂ shelled Co ₃ S ₄ hollow cubic heterostructure	1.58	10	[355]
MoS ₂ and Ni ₃ S ₂ heteronanorods grown on Ni foam	1.50	48	[45]
Co ₉ S ₈ and MoS ₂ nanohybrids	1.49	48	[356]
MoS ₂ shelled Co ₉ S ₈ heterostructures §	1.67	16	[14]
CoS ₂ , MoS ₂ and NiS ₂ heterostructured double shelled hollow polyhedron §	1.60	24	[357]
Co ₃ S ₄ /MoS ₂ heterostructured nanorods	1.66	30	[358]
Ni-Co complexes hybridized 1T-MoS ₂	1.44	48	[150]
Fe-Doped Co–Mo–S microtubes	1.605	60	[359]
Hydrangea-like Ni ₈ V ₂ (Mo ₃ S ₄) ₁₁ microspheres grown on Ni–Co foam	1.5@NA	-	[35]
Amorphous CoMoS ₄	1.72	12	[34]
Porous Ni–Mo–S nanowire network grown on Ni foam	1.54 2.0@100	12	[360]

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Hollow Fe doped Co–Mo sulfide heterostructures	1.6@20	10	[361]
N doped graphene encapsulated FeCoMoS nanoparticles §	1.58	40	[5]
1T/2H MoSe ₂ on Ti ₃ C ₂ nanosheets	1.64	50	[168]
Hollow CoSe ₂ nanocubes decorated with ultrathin MoSe ₂ nanosheets	1.524	12	[169]
Hierarchical MoSe ₂ and Ni _x Se _y nanosheets coated NiMoO ₄ nanorod grown on Ni foam (NiMoO ₄ /MoSe ₂ -Ni _x Se _y)	1.5	12	[173]
Ni ₃ Se ₂ /MoSe _x grown on Ni foam (Ni ₃ Se ₂ /MoSe _x)	1.57	12	[47]
NiSe/MoSe _x nanowires grown on Ni foam	1.91@100	14	[362]
Flower shaped hierarchical heterostructures of MoSe ₂ and WSe ₂ (MoSe ₂ /WSe ₂)	1.74	20	[171]
Heterostructure of La _{0.5} Sr _{0.5} CoO _{3-δ} and potassium ion bonded MoSe ₂ (La _{0.5} Sr _{0.5} CoO _{3-δ} /K-MoSe ₂)	1.59 1.95@100	2500	[174]
Ni doped MoSe ₂ and Ti ₂ NT _x nanosheet heterostructure (Ni–MoSe ₂ /Ti ₂ NT _x)	1.59	18	[172]
Mo carbides			
Mo ₂ C nanoparticles supported on carbon sheets	1.73	100	[200]
Mo ₂ C nanoparticles embedded in multichannel hollow C nanofibers	1.68	20	[363]
Mo ₂ C nanoparticles embedded in C nanosheets	1.65	30	[203]
N doped C wrapped Co nanoparticles and Mo ₂ C nanorods composite	1.68	~11.11	[364]
Mo ₂ C and Ni nanoparticles embedded in N doped porous C nanorods composite	1.66 1.79@50	10	[215]
Mo ₂ C embedded in N-doped carbon shelled Co nanoparticles	1.72	25	[365]
C layer confined hierarchical heterostructure of Mo ₂ C and Co nanoparticles grown on C cloth	1.67	12	[366]
Bamboo structured N doped CNT encapsulated Co and Mo ₂ C nanoparticles	~1.628	10	[217]
Mo ₂ C encapsulated Co nanoparticles embedded in carbonitride (Co-NC/Mo ₂ C)	1.685	20	[222]
Ni and Mo ₂ C nanoparticles embedded N-doped C nanofibers	1.64	100	[216]
Co/MoC nanoparticles embedded in C nanoboxes §	1.57	24	[367]
Co nanoparticles and Mo ₂ C decorated N doped C	1.67	30	[368]
Co ₉ S ₈ and Mo ₂ C nanoparticles anchored N and S doped C polyhedrons	1.61	20	[208]

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Mo ₂ C anchored N doped CNTs encapsulated NiS ₂ (N-CNT/NiS ₂ @Mo ₂ C)	1.52	24	[212]
Porous graphene shell encapsulated Co ₂ P/Mo ₂ C/Mo ₃ Co ₃ C nanoparticles	1.74	10	[224]
B,N doped Mo ₂ C nanoparticles imbedded in B,N doped carbon network (B,N:Mo ₂ C@BCN)	1.84@100	20	[225]
Mo ₂ C nanoparticles embedded in N-doped graphene shell encapsulated Co _x Fe _y alloy nanoparticles (Mo ₂ C-NC@Co _x Fe _y)	1.53 1.60 V@ 20	16	[221]
Co ₆ Mo ₆ C ₂ /Co ₂ Mo ₃ O ₈ nanoparticles dispersed N,P doped reduced graphene oxide	1.81	~13	[369]
Co doped Mo ₂ C nanorods encapsulated N doped graphitic carbon shell	1.67	12	[370]
N doped CNT encapsulated Ni/MoC heteronanoparticles	1.535	30	[229]
Mo _x C and Ni nanoparticles anchored N-doped graphene CNT hybrid (Ni-Mo _x C/NC-100)	1.72	-	[228]
MoC ₂ -doped NiFe alloy nanoparticles encapsulated N-doped graphene (NG-NiFe@MoC ₂)	1.53	10	[31]
N doped C encapsulating Co and Mo _x C nanoparticles	1.74	6	[371]
Vertically aligned Mo ₂ C nanosheets on Co nanoparticles embedded in N doped C polyhedron §	1.62	-	[372]
N doped C wrapped Co-Mo ₂ C heterostructure	1.68	20	[373]
Mo oxides			
Porous MoO ₂ nanosheets grown on Ni foam	1.53	24	[253]
P,W doped MoO ₂ nanoflowers grown on Ni foam	1.65@30	20	[42]
N-doped-graphene encapsulated Ni nanoparticles coupled with MoO ₂ nanosheets grown on Ni foam (Ni@C-MoO ₂ /NF)	1.54	196	[264]
NiFeP-MoO ₂ hybrid nanorods grown on Ni foam	1.41 1.65@100	550	[374]
Nanorod heterostructure of MoO ₂ , MoS ₂ , Co ₉ S ₈ and C	1.62	20	[48]
Porous NiMoO _{4-x} /MoO ₂ hybrid grown on Ni foam	1.56	~16.67	[89]
Ultrafine Ni and MoO ₃ nanoparticles coupled with amorphous NiO nanosheets grown on carbon cloth (MoO ₃ /Ni-NiO)	1.55	20	[49]
Ni(PO ₃) ₂ -MoO ₃ nanorods (Ni(PO ₃) ₂ /MoO ₃) grown on Ni foam	1.47	~8.33	[277]
NiS nanosheets decorated MoO ₃ nanorods grown on Ni foam	1.56	20	[278]
Hierarchical <i>in situ</i> grown Prussian blue analogue phosphide anchored on Ni ₂ P@MoO _x nanosheet spheres grown on Ni foam (IPBAP)	1.494	-	[281]

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HER/OER Catalyst	Full cell voltage (V) @10 mA cm ⁻² except for special noting	Cell stability test (h)	Ref.
Hierarchical heterostructure of CoMoO ₄ nanosheets and NiCo ₂ O ₄ nanowires grown on Ni foam (NiCo ₂ O ₄ @CoMoO ₄ /NF)	1.55	12	[50]
N doped NiMoO ₄ nanowires and NiS ₂ nanosheets heterostructure grown on carbon fiber cloth (N-NiMoO ₄ /NiS ₂)	1.60	20	[285]
CoP ₃ and NiMoO ₄ nanosheet heterostructure (CoP ₃ /NiMoO ₄) grown on Ni foam	1.57	12	[286]
NiC/MoC/NiMoO ₄ heterostructured nanorod arrays grown on Ni foam	1.52	20	[375]
	1.50		
Ni nanoparticles decorated MoO ₂ /NiMoO ₄ microrod arrays grown on Ni foam	1.66@50 1.76@100	87	[376]
	1.50		
Porous nanoplate array of Ni network coupled Ni-Fe-Mo suboxide grown on Ni foam (Ni/NiFeMoO _x /NF)	1.63@100	100	[287]
Amorphous Co-Mo-P-O grown on Ni foam	1.57	80	[377]
Co-Mo-V layered double hydroxide nanosheet (CoMoV-LDH) grown on Ni foam	1.61	20	[301]
Mo nitrides			
	1.498@20		
NiMoN nanowires with (100) exposed facet grown on Ni foam	1.532@50 1.559@100	50	[36]
	1.576		
Metallic Co attached Mo ₂ N tubes (Co-Mo ₂ N)	1.671@20 1.832@50	44	[315]
Ni-Mo nitride nanotubes	1.596	30	[309]
NiMoN _x nanorods grown on Ni foam	1.49	110	[316]
CoMoN _x nanosheet arrays grown on Ni foam	1.55	100	[321]
Nanosheets composed hierarchically porous Co doped NiMoN nanowires (Co-NiMoN-400 NR) §	1.57	20	[323]
N-doped CNT encapsulated Ni/MoN heterostructures grown on carbon cloth	1.699	24	[317]
NiMoN nanowire arrays grown on Ni foam	1.507	35	[37]

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HER/OER Catalyst	Full cell voltage (V) @10 mA cm ⁻² except for special noting	Cell stability test (h)	Ref.
Hierarchical Ni-Fe-MoN porous nanotubes (Ni-Fe-MoN NTs) §	1.513	45	[82]
Mo phosphides			
Hierarchical MoP nanoflake array grown on Ni foam	1.62	20	[378]
MoP nanosheets on Ni ₃ P grown on Ni foam	1.67	45	[379]
NiMoP ₂ nanowires grown on C cloth	1.67	24	[331]
Hierarchical NiMo phosphide nanosheets anchored on CNT (Ni ₁ Mo ₁ P NSs@MCNTs)	1.601	36	[332]
Mo borides			
Co-Mo-B nanoparticles	1.69 (1 M NaOH)	25	[380]
Mo alloys			
Mo–Ni alloy nanoparticles	1.62 1.72@20	24	[32]
Ni–Mo shelled Cu nanowires grown on Cu foam	1.61	12	[337]
Ni-Fe-Mo alloy grown on Ni foam	1.45	50	[339]
Network like Ni _{0.75} Mo _{0.25} nanosheets grown on C cloth	1.74	10	[381]
NiMo hollow nanorod array grown on Ti mesh (NiMo HNRs/TiM)	1.64	10	[338]
Ni–Mo alloy microsphere films grown on Cu foil	1.59	110	[33]
Ni-Fe-C-Mo film grown on Ni mesh	1.61	12	[382]
NiMoCo hybrid nanowire arrays grown on Ni foam (NF@NiMoCo)	1.56	100	[341]

Table S2 OER/OER bifunctionality of Mo-based catalysts in 0.1 M KOH (except for special noting)
Metal-air battery stability test: Non-aqueous electrolyte (except for special noting)
Voltage (V) values are calculated with respect to reversible hydrogen electrode (RHE) unless specified
§ denotes HER/OER/ORR trifunctional catalysts

OER/ORR Catalyst	OER $E_{j=10}$ @10 mA cm ⁻² (V)	ORR $E_{1/2}$ or E_{-3} (V)	$\Delta E = \text{OER } E_{j=10} -$ ORR $E_{1/2}$ or E_{-3} (V)	Metal-air battery stability test: cycle no. and time	Ref.
Mo chalcogenides					
1T-MoS ₂ and functionalized CNT hybrid	1.52	0.81	0.71	100, -	[108]
N doped MoS ₂	1.56 (1.0 M KOH)	0.81	-	224, -	[29]
Vertically aligned MoS ₂ nanosheet encapsulated N doped C framework (Mo- N/C@MoS ₂) §	~1.5	0.81	0.69	12, 48 h (6.0 M KOH with 0.2 M zinc acetate)	[151]
MoS ₂ and CoP heterostructure loaded on N, P-doped C §	1.536 (1.0 M KOH)	0.79	-	300, - (6.0 M KOH with 0.2 M zinc acetate)	[354]
Co and Nb doped MoS ₂ nanosheets shelled micro-TiO ₂ hollow spheres §	1.49 (1.0 M KOH)	0.87	-	-	[353]
MoS ₂ shelled Co ₉ S ₈ heterostructures §	1.572 (1.0 M KOH)	~0.78	-	120, 20 h (6.0 M KOH with 0.2 M zinc acetate)	[14]
CoS ₂ , MoS ₂ and NiS ₂ heterostructured double shelled hollow polyhedron §	1.43 (1.0 M KOH)	0.80	-	~, 40 h (NA)	[357]
Co ₉ S ₈ quantum dots and MoS ₂ embedded in N doped C nanoflake arrays grown on C nanofiber §	0.57 (1.0 M KOH)	0.82	-	120, 50 h	[13]
Mo carbides					
Mo ₂ C shelled C hybrid microspheres (Mo ₂ C-C)	1.589	0.713	0.876	-	[197]
MoS ₂ shelled Mo ₂ C nanoparticles	1.51	0.60	0.91	-	[28]
N doped graphene encapsulated Mo ₂ C, Co nanoparticles embedded in N doped C (Mo ₂ C@NC/Co@NG). §	1.653	0.867	0.786	480, 80 h	[220]
N-doped carbon encapsulated Co and MoC heterojunction nanoparticles	1.52 (1.0 M KOH)	0.824	-	80, 28.3 h	[234]
Co nanoparticles tipped N doped CNTs attached house centipede-like MoC-Mo ₂ C nanorods (MoC-Mo ₂ C/NCNT)	1.67	0.80	0.87	162, -	[6]
Co ₆ Mo ₆ C ₂ and metallic Co attached N doped C composite with nanorod morphology (Co ₆ Mo ₆ C ₂ -Co@NC)	1.498 (1.0 M KOH)	0.803	-	1800, 300 h (6.0 M KOH with 0.2 M zinc acetate)	[242]
N doped rGO covered metal Co and Mo ₂ C composite nanoparticles	1.56 (1.0 M KOH)	0.178 vs. Ag/A gCl	-	-	[383]
Co, Zn, N doped CNT arrays branched N- doped carbon frameworks encapsulated MoC nanowires	1.675	0.914	0.761	780, 130 h (6.0 M KOH with 0.2 M zinc chloride)	[384]
Co/MoC nanoparticles embedded in C nanoboxes §	~1.5	0.875	0.625	~, 100 h (6.0 M KOH with 0.2 M zinc acetate)	[367]
Vertically aligned Mo ₂ C nanosheets on Co nanoparticles embedded in N doped C polyhedron §	~1.51 (1.0 M KOH)	0.84	-	~, 190 h (6.0 M KOH with 0.2 M zinc acetate)	[372]

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OER/ORR Catalyst	OER $E_{j=10}$ @10 mA cm ⁻² (V)	ORR $E_{1/2}$ or E_{-3} (V)	$\Delta E = \text{OER } E_{j=10} -$ ORR $E_{1/2}$ or E_{-3} (V)	Metal-air battery stability test: cycle no. and time	Ref.
Mo oxides					
MoO ₃ nanosphere embedded in rGO (GMS)	-	0.53	-	-	[279]
MoO _x and NiO mixed oxide nanoparticles with C support (Mo-Ni)	1.70	0.74	0.96	-	[282]
P doped SrCo _{0.5} Mo _{0.5} O ₃ microstructure	~1.68	~0.72	0.96	-	[289]
Mo nitrides					
Hierarchical Ni-Fe-MoN porous nanotubes (Ni-Fe-MoN NTs) §	1.53	0.72	0.81	~, 20 h (6.0 M KOH with 0.2 M zinc acetate)	[82]
Co ₃ Mo ₃ N mesoporous nanostructures	~0.72 vs. Ag/AgCl	-	-	10, -	[39]
Mo phosphides					
MoP _x and MnP _y heteronanoparticle attached mesoporous N, P doped graphene (MnP _x @MoP _y /N,P-Gr) §	1.54@20	0.842	-	-	[333]