The synthesis of W-Ni_3S_2/NiS nanosheets with heterostructure as high efficiency catalyst for urea oxidation

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Chemicals and reagents

The nickel foam (NF, thickness 1.0 mm) was obtained by Kunshan Guangjiayuan New Material Co., Ltd; The thioacetamide (TAA,CH_3CSNH_2) from Sarn Chemical Technology (Shanghai) Co., Ltd; The sodium tungstate (Na_2WO_4) from Tianjin Sinopharm Chemical Reagent Factory.; Polyvinylpyrrolidone (PVP) from Tianjin Guangfu Fine Chemical Research Institute; potassium hydroxide (KOH) from Tianjin Damao Chemical Reagent Factory; Urea ($CO(NH_2)_2$ from Tianjin Damao Chemical Reagent Factory; Concentrated hydrochloric acid (HCl, 12 mol/L) was bought from Chengdu Cologne Chemical Co., LTD.

DFT computation details:

The DFT calculations were performed using the Cambridge Sequential Total Energy Package (CASTEP) with the plane-wave pseudo-potential method. The geometrical structures of the (220) plane of W-Ni_3S_2, and the (110) plane of NiS was optimized by the generalized gradient approximation (GGA) methods. The Revised Perdew-Burke-Ernzerh of (RPBE) functional was used to treat the electron exchange correlation interactions. A Monkhorst Pack grid k-points of 6*8*1 and 5*6*1 of W-Ni_3S_2 and NiS, a plane-wave basis set cut-off energy of 500 eV were used for integration of the Brillouin zone. The structures were optimized for energy and force convergence set at 0.05 eV/A and 2.0×10^{-5} eV, respectively.

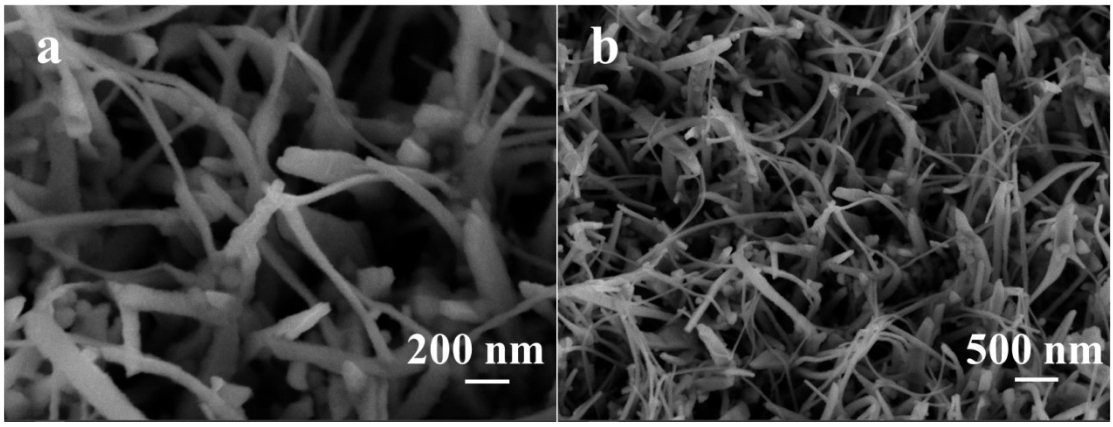

Fig.S1 SEM images of W-Ni_3S_2.

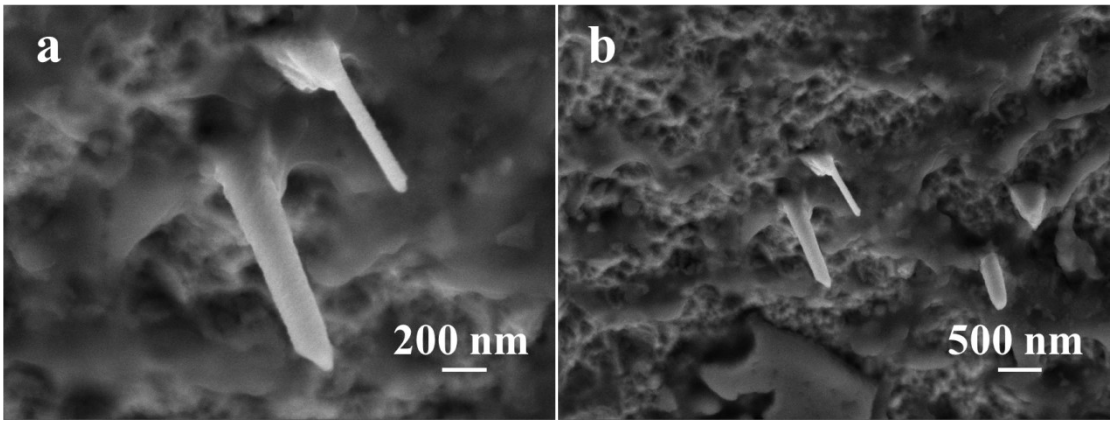

Fig.S2 SEM images of Ni_3S_2.

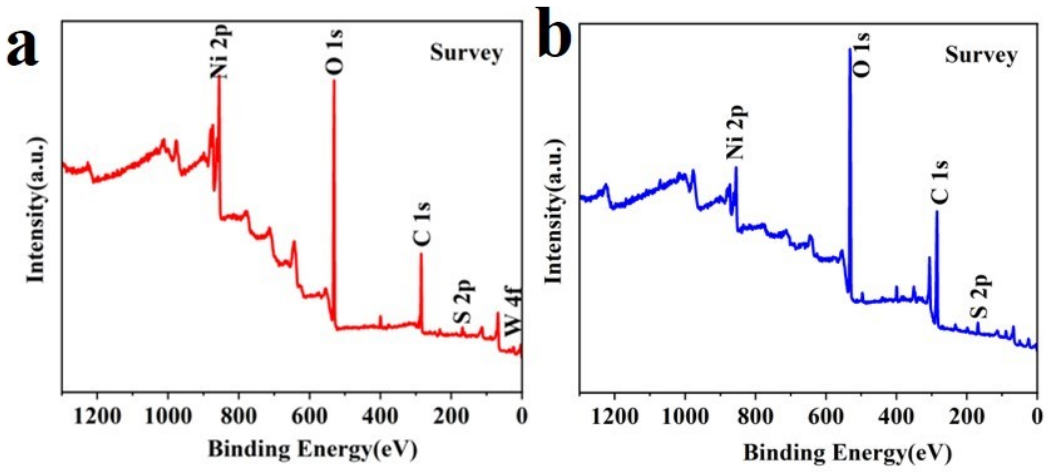

Fig.S3 Survey of a) W-Ni_3S_2/NiS, b) Ni_3S_2.

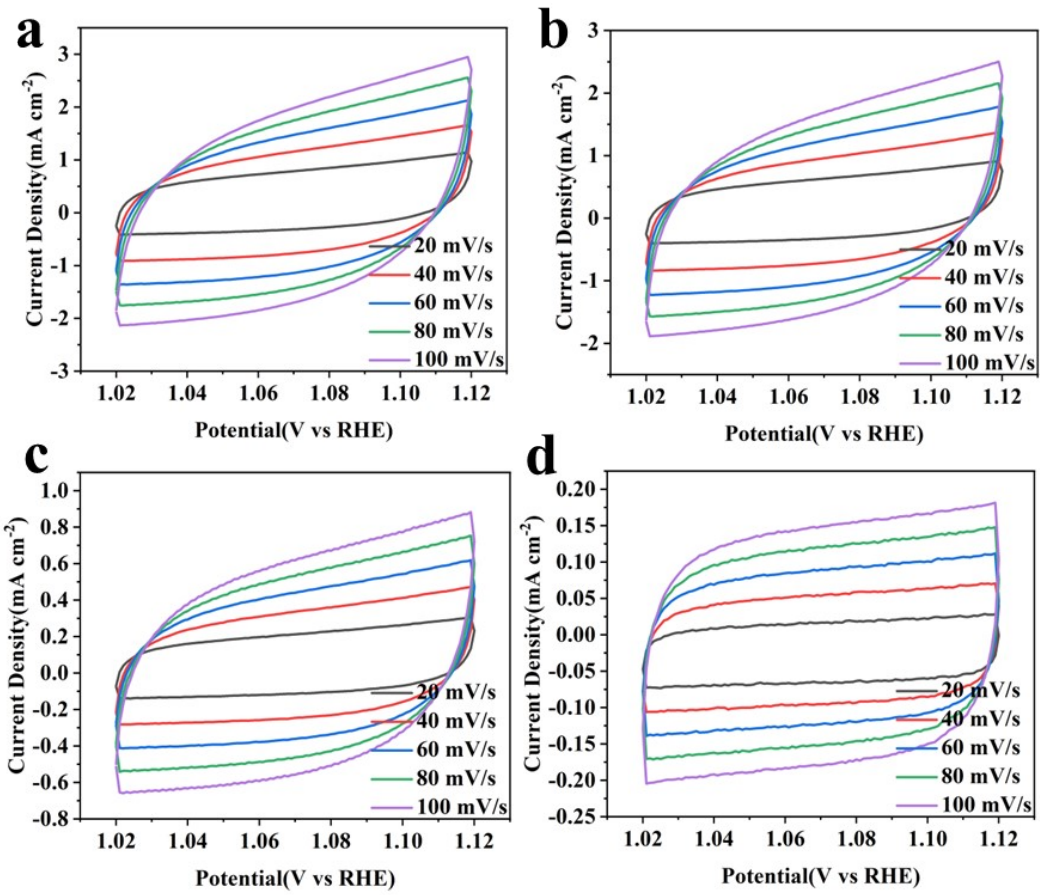

Fig.S4 CV plots of a) W-Ni_3S_2/NiS, b) W-Ni_3S_2, c) Ni_3S_2, d) NF at different scan rates.

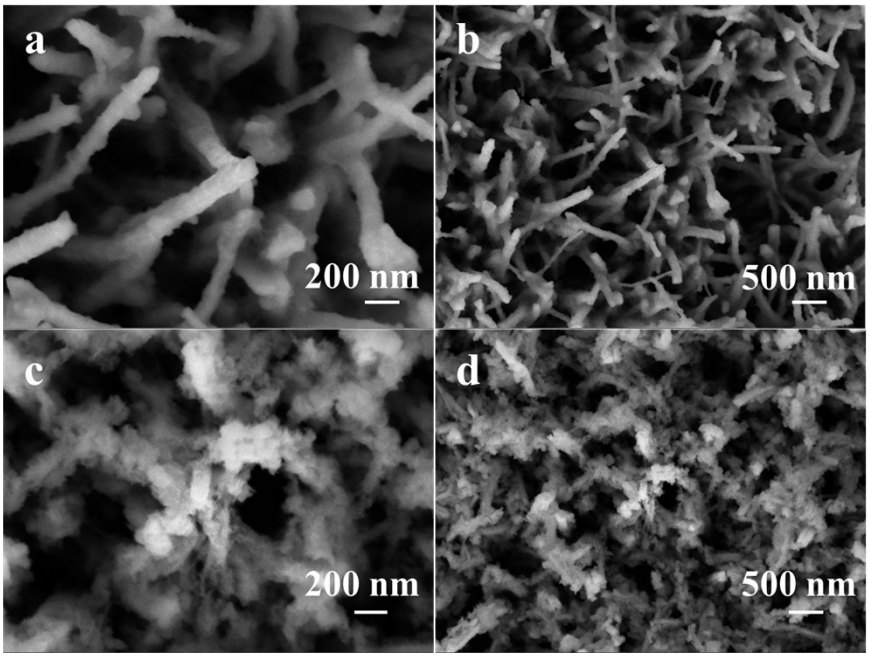

Fig.S5 SEM images of W-Ni_3S_2/NiS before(a-b)and after(c-d)stability test.

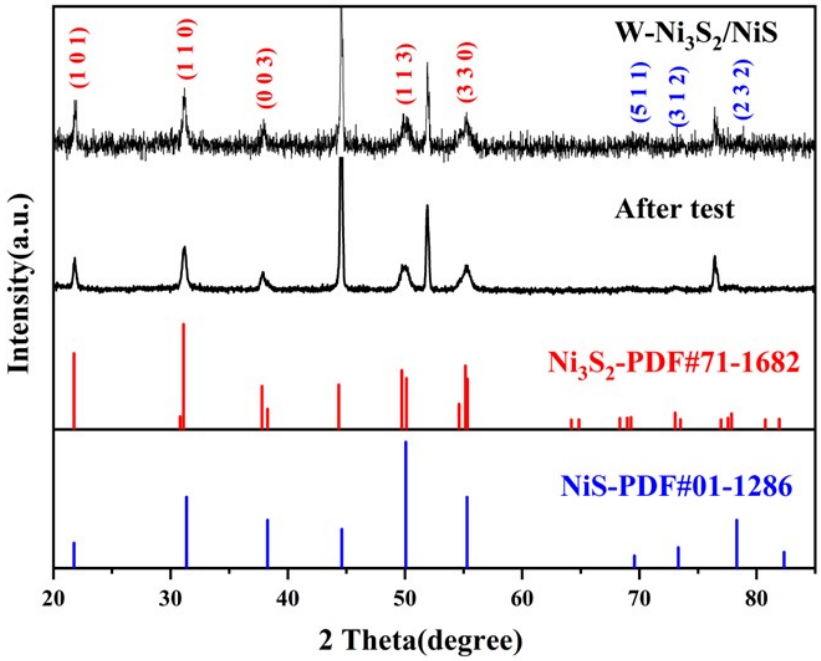

Fig.S6 XRD patterns of W-Ni_3S_2/NiS before and after stability test.

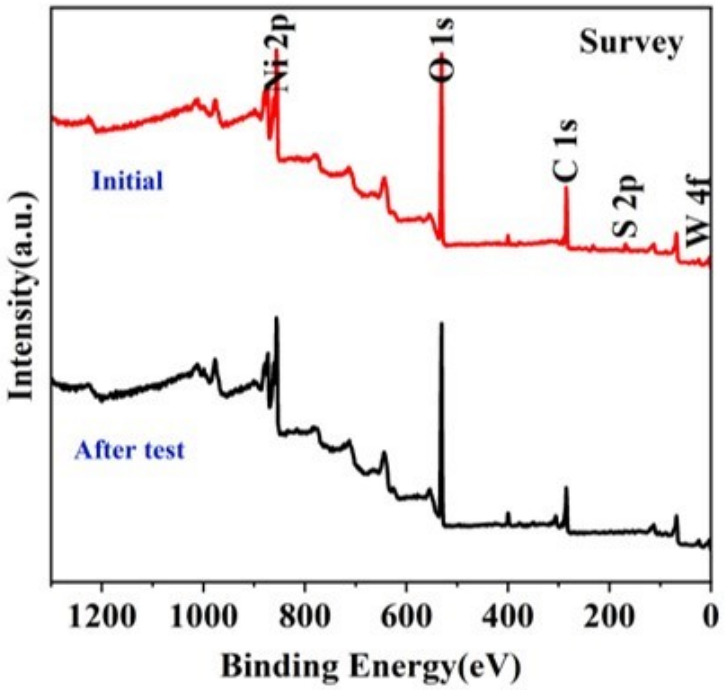

Fig.S7 XPS of W-Ni_3S_2/NiS before and after stability test.

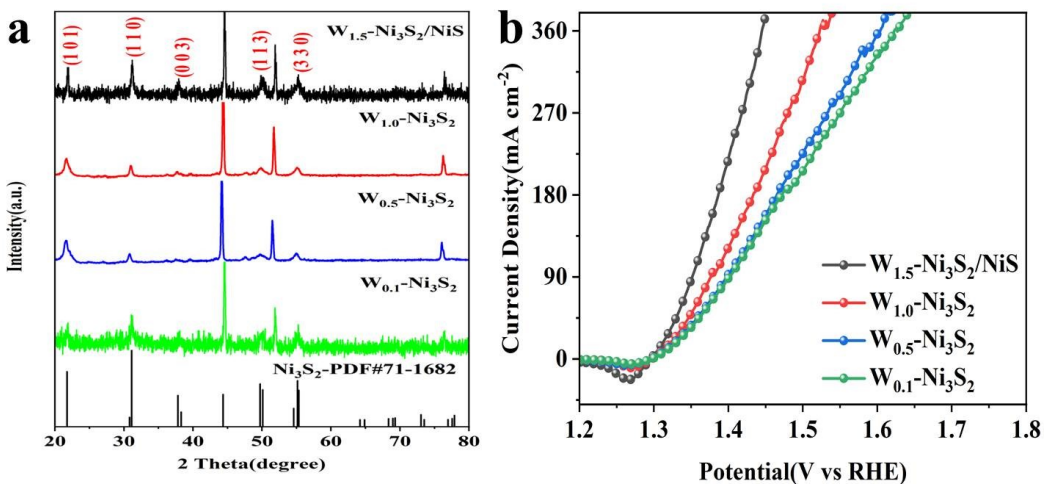

Fig. S8 XRD (a) and UOR (b) performance of as prepared materials.

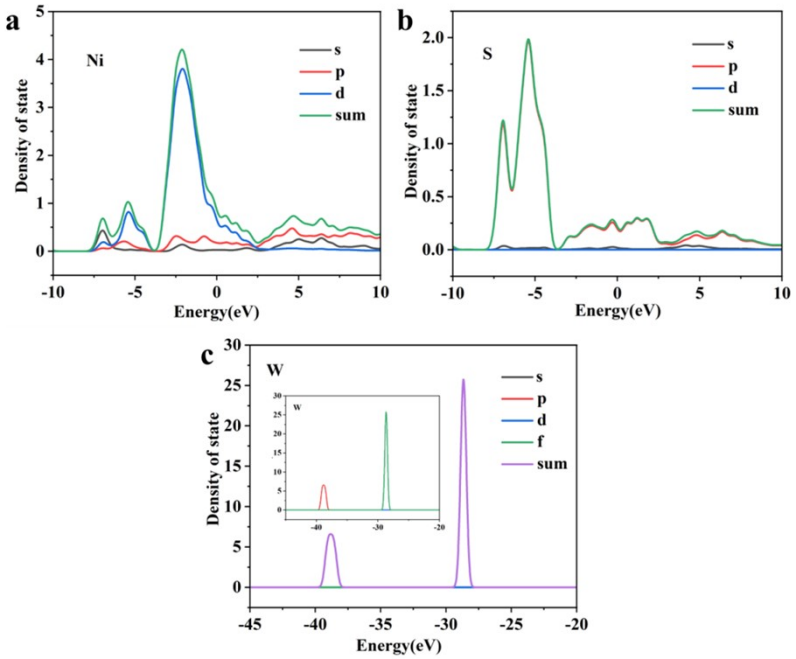

Fig. S9 Density of states for W-Ni_3S_2, (a) Ni, (b) S and (c) W.

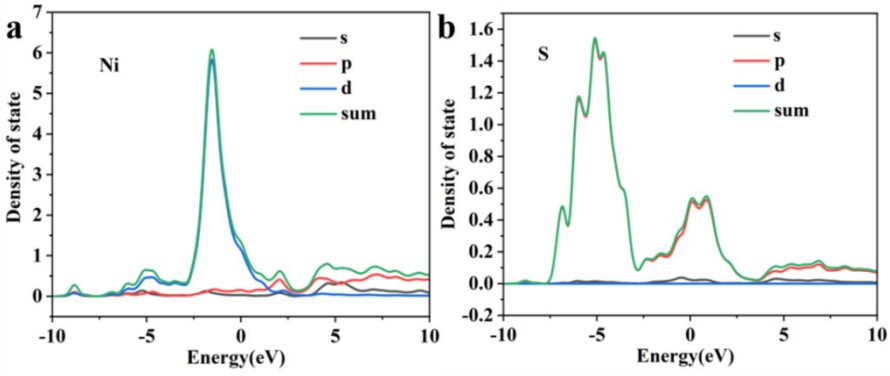

Fig. S10 Density of states for NiS, (a) Ni and (b) S.

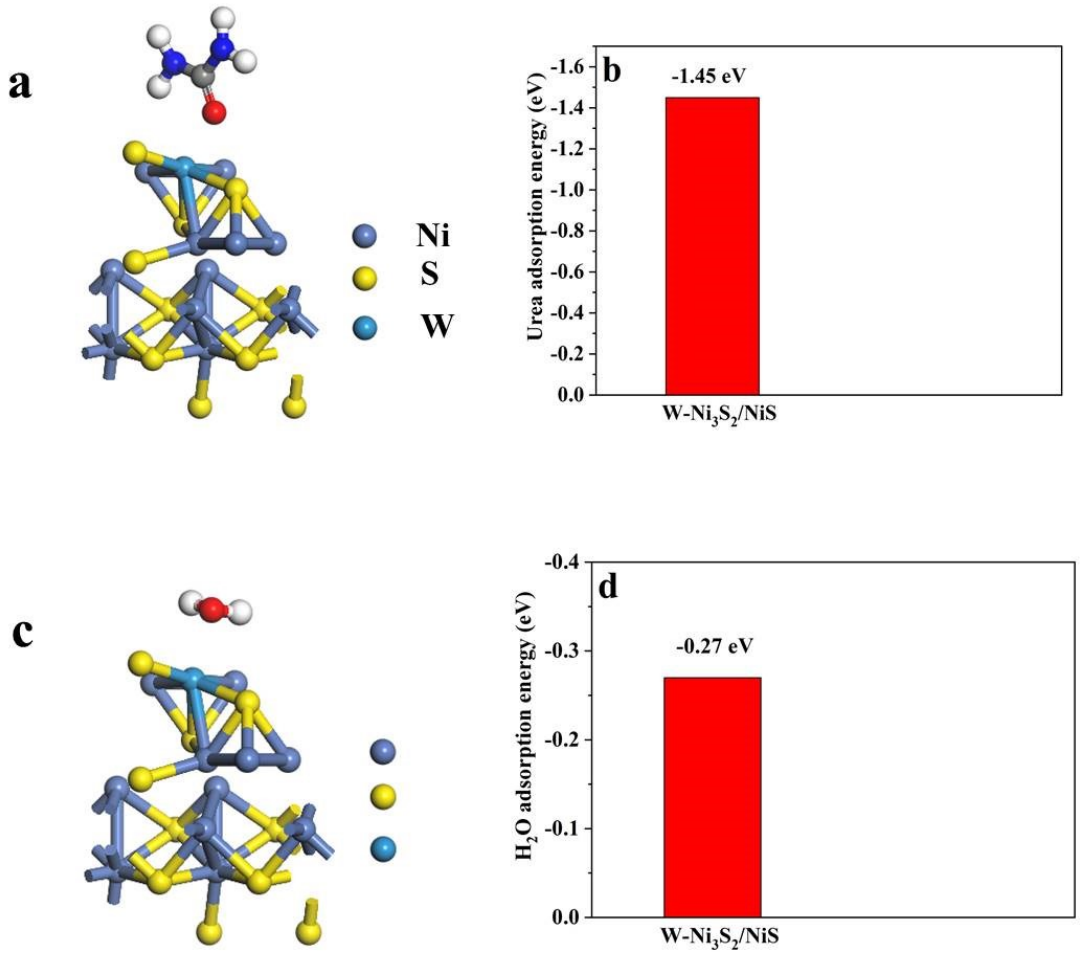

Fig. S11 The ball-and-stick model of urea adsorbed on (a) W-Ni_3S_2/NiS and (b) Urea adsorption energy; the ball-and-stick model of H_2O adsorbed on (c) W-Ni_3S_2/NiS and (d) H_2O adsorption energy.

Table S1 Comparison of charge transfer resistance (R2) values of all samples in alkaline solution (UOR).

catalyst	R2(Ω)
W-Ni_3S_2/NiS	**0.895**
W-Ni_3S_2	1.088
Ni_3S_2	1.304
NF	$5.584*10^{16}$

Table S2 Comparisons of UOR activity of non-noble-metal electrocatalysts.

catalysts	Electrolytes	Potential(V)	Reference
W-Ni_3S_2/NiS	**1M KOH+0.5M urea**	**1.309 V**	**This work**
Ni_3S_2@MoS_2 CS	1M KOH+0.5M urea	1.336 V	[1]
Mn-NiS_x/NiO/Ni_3N	1M KOH+0.5M urea	1.35 V	[2]
FeCo-LDH	1M KOH+0.5M urea	1.328 V	[3]
Ce-Ni_3N@CC	1M KOH+0.5M urea	1.31 V	[4]
FeMn-PS	1M KOH+0.33M urea	1.33 V	[5]
O-NiMoP/NF	1M KOH+0.5M urea	1.31 V	[6]
Mn-Ni_3S_2/NF	1M KOH+0.5M urea	1.30 V	[7]
Mo-doped Ni_3S_2	1M KOH+0.3M urea	1.33 V	[8]
MOF-Ni@MOF-Fe–S	1M KOH+0.5M urea	1.347 V	[9]
VOOH-Ni	1M KOH+0.33M urea	1.356 V	[10]

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