

### Supplementary information

#### **Integrating FeS<sub>2</sub> nanospheres on hexagonal Boron nitride: A Nanomolar Detection and visible-light-driven photoreduction of Cr (VI)**

Irfan Nazir<sup>a</sup>, Firdous Ahmad Ganaie<sup>a</sup>, Aaliya Qureashi<sup>a</sup>, Zia Ul Haq<sup>a</sup>, Arshid Bashir<sup>a,b</sup>, Abdullah Yahya Abdullah Alzahrani<sup>c</sup>, Altaf Hussain Pandith<sup>a,d\*</sup>

<sup>a</sup> *Laboratory of Nanoscience and Quantum Computations, Department of Chemistry, University of Kashmir, Hazratbal, Srinagar-190006, Kashmir, India*

<sup>b</sup> *Department of Chemistry, Govt. Degree college, Beerwah-193411, Budgam, J&K, India*

<sup>c</sup> *Department of Chemistry, Faculty of Science & Arts- Muhail Asser, King Khalid University- 61413, Saudi Arabia*

<sup>d</sup> *Lucent Institute of Excellence and Child Care, Sopore-193201, J&K, India*

#### **\*Corresponding Author**

##### **Prof. Altaf Hussain Pandith**

Department of Chemistry  
University of Kashmir  
Srinagar-190006  
India

Phone: +91-194-2424900(OFFICE)  
+91-7006429021 (Mobile)  
Fax: +91-194-2414049  
E-mail: [altafpandit23@gmail.com](mailto:altafpandit23@gmail.com)

## **1. Materials used**

The experiments used iron trichloride, thiourea, urea, and boric acid. All the chemicals used in the study were analytical grade and obtained from Sigma-Aldrich & Merck. Ultrapure fresh water, obtained from a Millipore water purification system, was used.

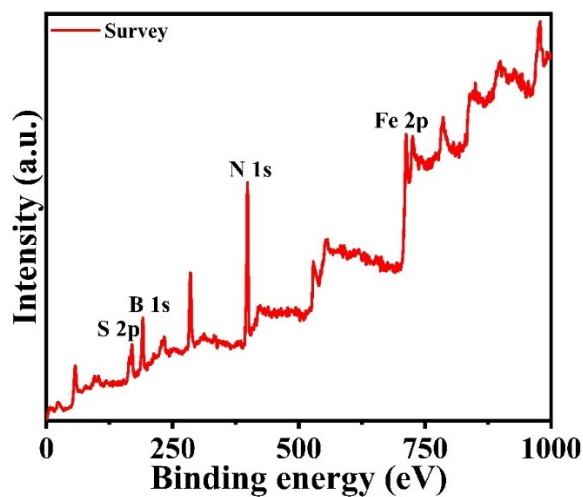
## **2. Fabrication of the modified electrode**

A modified glassy carbon electrode (GCE) was created using the drop-casting method with a heterostructure of h-BN-FeS<sub>2</sub> and pristine h-BN and FeS<sub>2</sub>. This modified GCE was used as the working electrode for detecting Cr (VI) electrochemically. Before the surface modification, the GCE was cleaned by sonication with distilled water and then polished with 0.1  $\mu\text{m}$  alumina powder. The sample suspension was made homogenous by sonicating it in dimethylformamide (DMF) at a concentration of 3 mg mL<sup>-1</sup> for 10 minutes and then drop-casted (approximately 5  $\mu\text{L}$ ). Additionally, the GCEs were left to dry overnight at room temperature. For the electrochemical experiments, 0.1 M KNO<sub>3</sub> and 0.1 M HCl were used as the supporting electrolytes. All the experiments, such as CV, LSV, DPV, and chronoamperometry, were carried out using the same parameters

## **3. Instrumentation and methods**

Various methods and instrumentation were employed to explore the potential properties of the synthesised material for electrochemical sensing applications and to characterise it. Field emission scanning electron microscopy (ZEISS Gemini FE-SEM) and energy-dispersive X-ray spectrometry (Octane Elect EDS) were used to investigate the surface morphology and the elemental composition of the synthesised materials. Rigaku's Smart Lab X-ray diffractometer was used to determine the crystal structure and phase configuration. X-ray photoelectron spectroscopy was used to examine the material's chemical makeup and valence states quantitatively, using a Physical Electronics Versa Probe III system. A three-electrode cell with a conventional biological potentiostat electrocatalytic workstation was used to conduct EIS measurements. In this experiment, a conventional three-electrode cell was used, modified GCE (surface area = 0.072 cm<sup>2</sup>), Saturated Ag|AgCl, and Pt wire being used as the working,

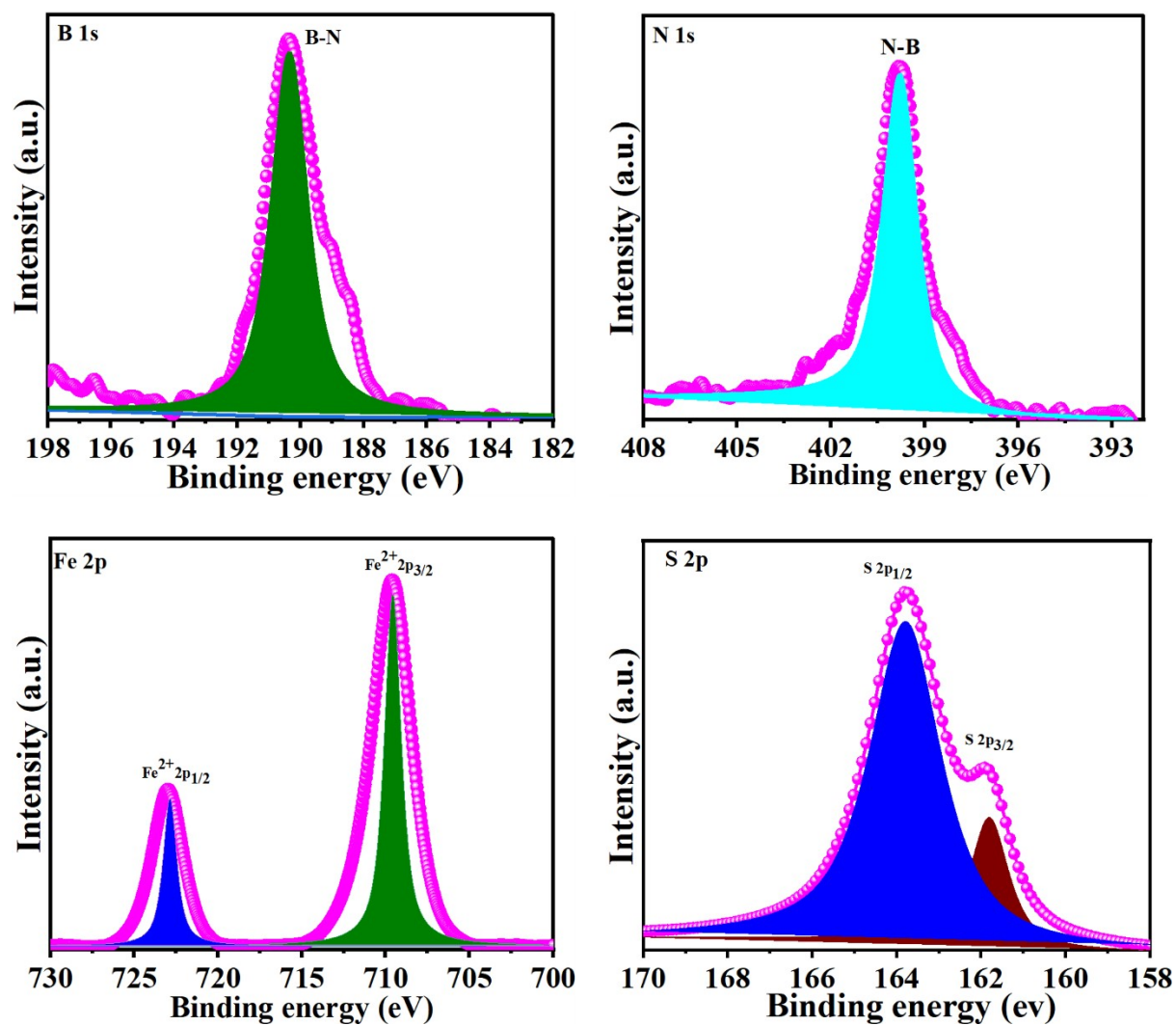
reference, and counter electrodes, respectively. Zeta potential investigations were conducted on the Anton Paar Lite Sizer 500.



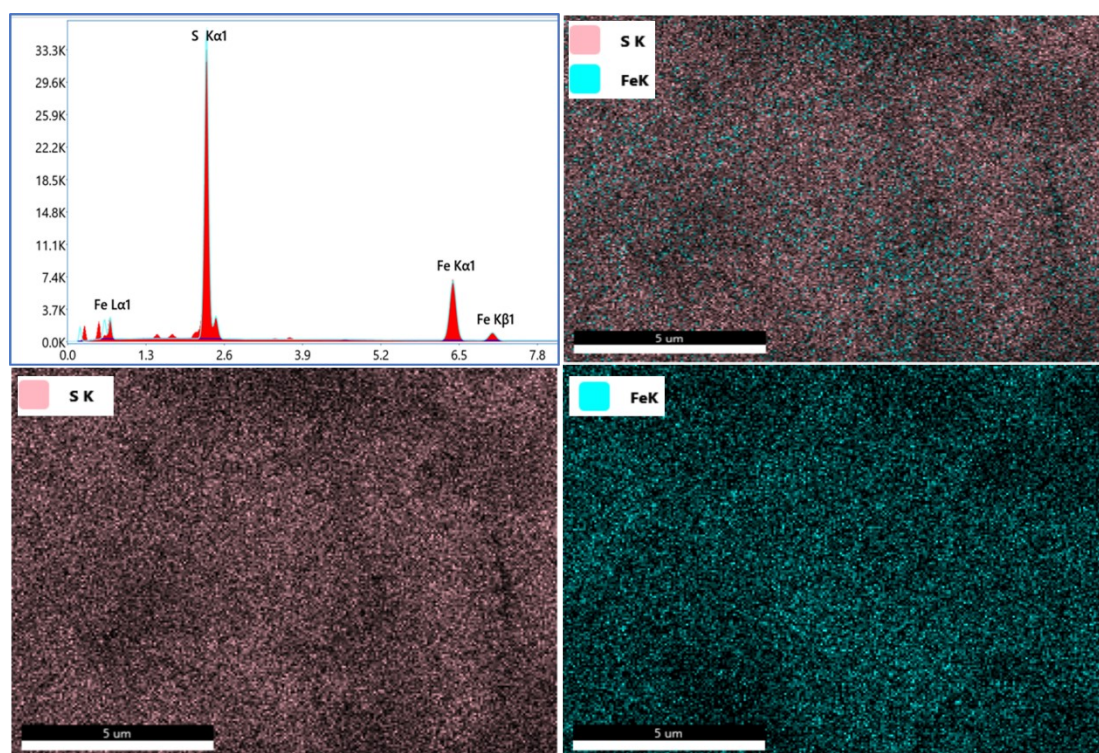
**Fig.S1** XPS survey scan of h-BN/FeS<sub>2</sub>

**Table S1** Sensing of Cr (VI) in the natural samples by using the sensor h-BN/FeS<sub>2</sub>/GCE

Sample	Cr (VI) (Real) $\mu\text{A}$	(Unspiked) $\mu\text{A}$	(Spiked) $\mu\text{A}$	Recovery factor (%)
Dal Water	-7.4	-33.1	-106.4	99
Sewage water	-7.4	-32.6	-95.2	84.5

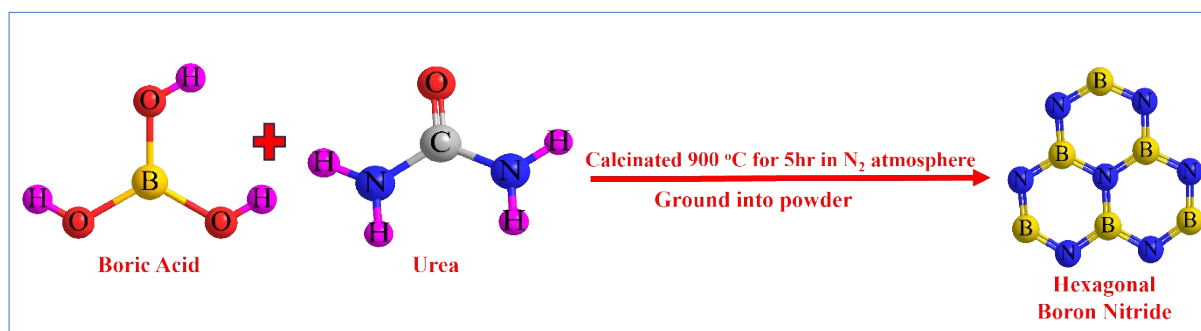


**Fig.S2** High-resolution XPS survey scan of pristine h-BN and  $\text{FES}_2$



**Fig.S3.** EDS spectra of FeS<sub>2</sub> and elemental mapping micrographs of FeS<sub>2</sub>

Elemental mapping micrographs show that iron and sulphur are uniformly distributed and EDS spectra depict that iron and sulphur are present in the same ratio as set in the reaction.

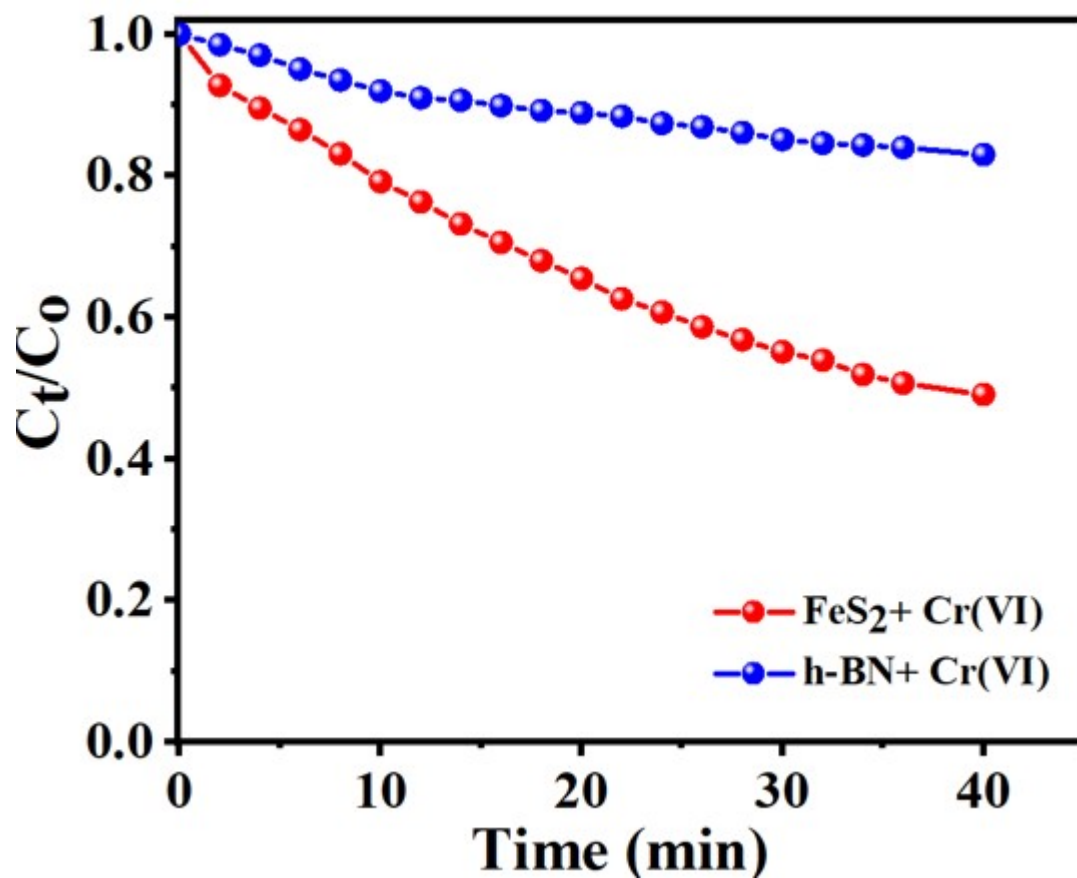


**Scheme S1** Schematic illustration of the synthesis of h-BN

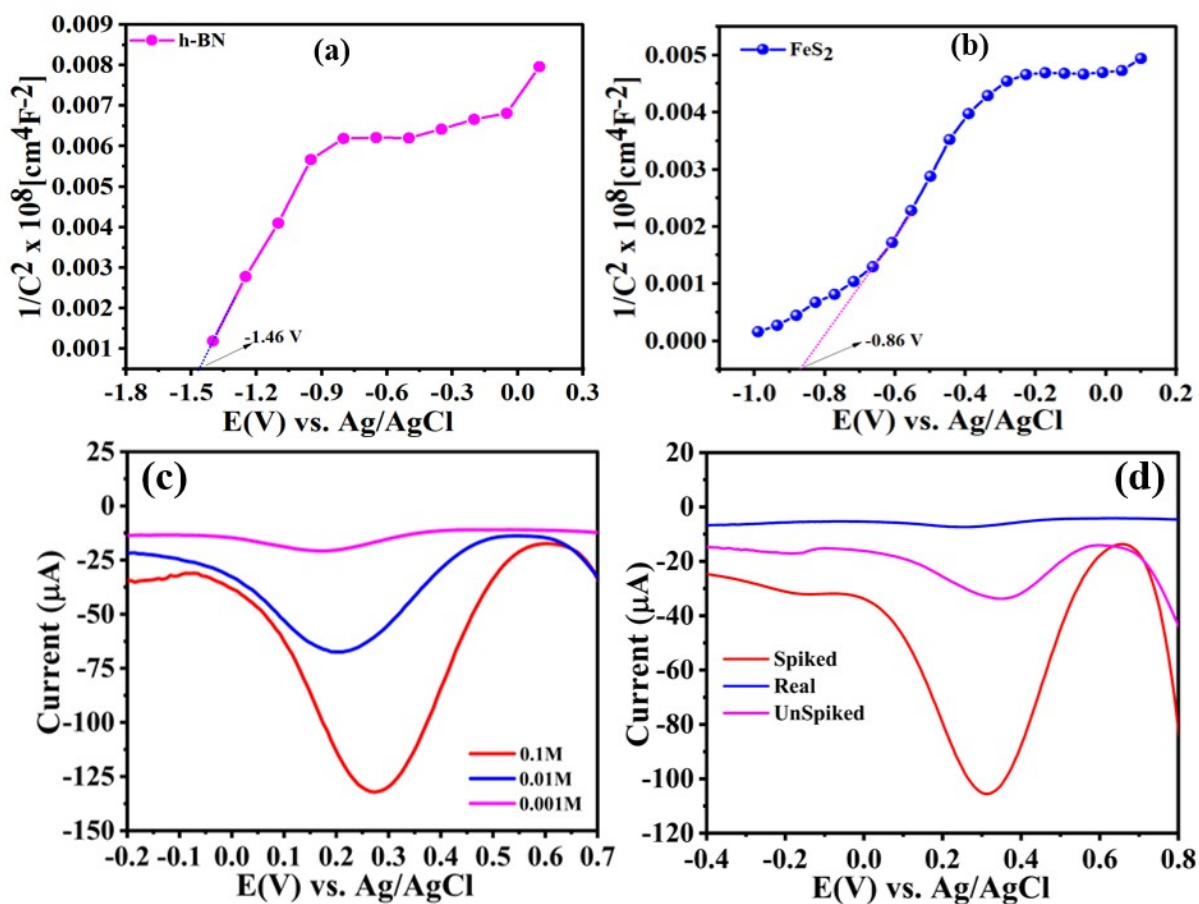
**Tauc's formula**

$$(\alpha h\nu)^n = k(h\nu - E_g) \quad 1$$

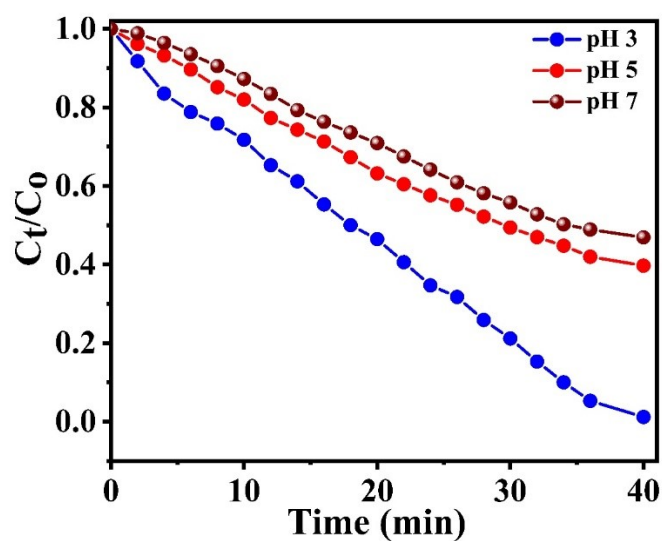
The absorption coefficient, light frequency, and Planck's constant are represented by  $\alpha$ ,  $\nu$ , and  $h$ , respectively. In the case of a direct semiconductor,  $n=2$ , while  $n=1/2$  for an indirect semiconductor.



**Fig.S4** Adsorption studies of the h-BN/FeS<sub>2</sub> catalyst for the reduction of Cr (VI) in the presence of FeS<sub>2</sub> and h-BN.



**Fig.S5** Mott–Schottky curves of (a) h-BN and (b) FeS<sub>2</sub> (c), DPV of 50 μM Cr (VI) at the h-BN/FeS<sub>2</sub> /GCE in 0.001, 0.01 and 0.1 M HCl solutions at a scan rate of 50 mVs<sup>-1</sup>. (d) DPV profiles of different real samples using h-BN/FeS<sub>2</sub> /GCE containing Cr (VI) in Dal Lake water.



**Fig.S6** Effect of pH on the photocatalytic reduction of Cr (VI)



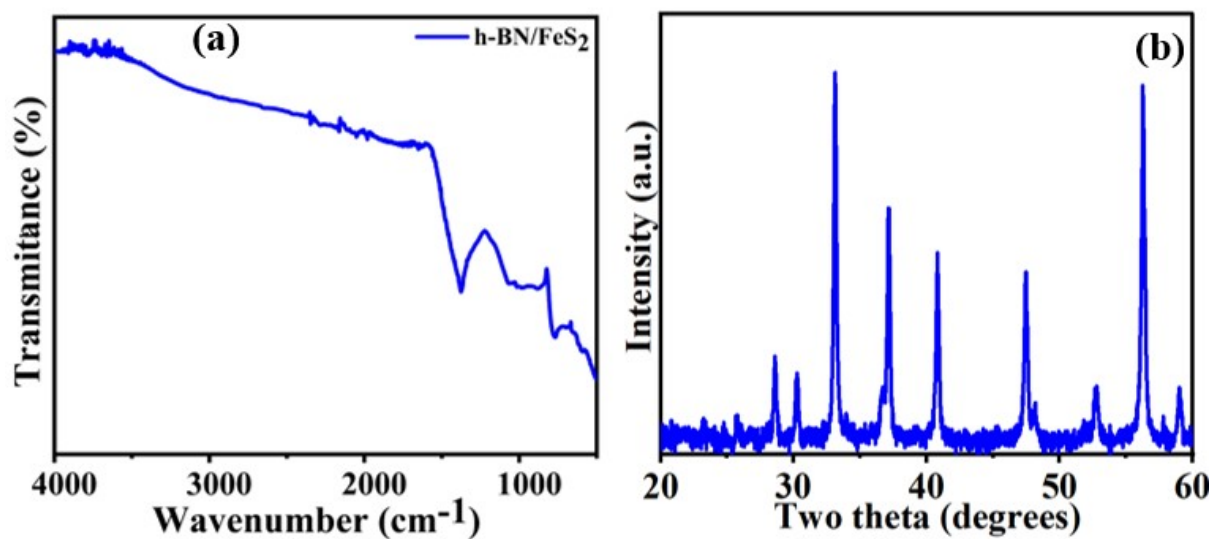


Fig.S7 FTIR spectra and XRD pattern of h-BN/FeS<sub>2</sub> after the catalysis

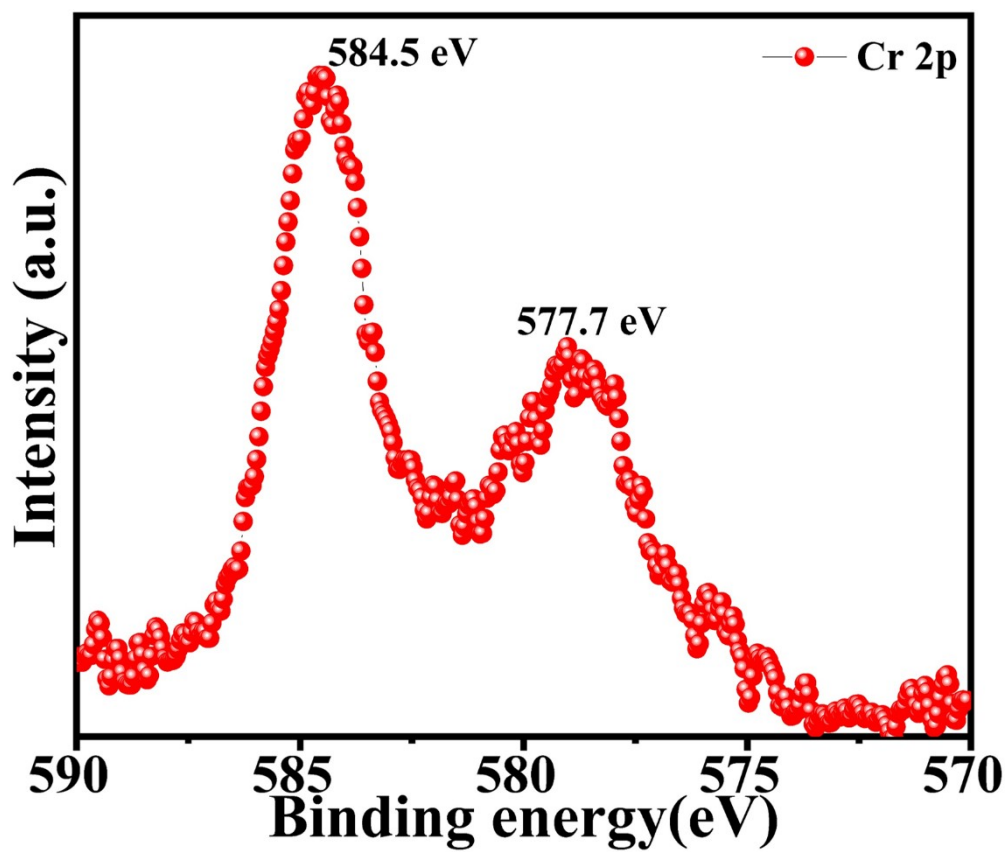
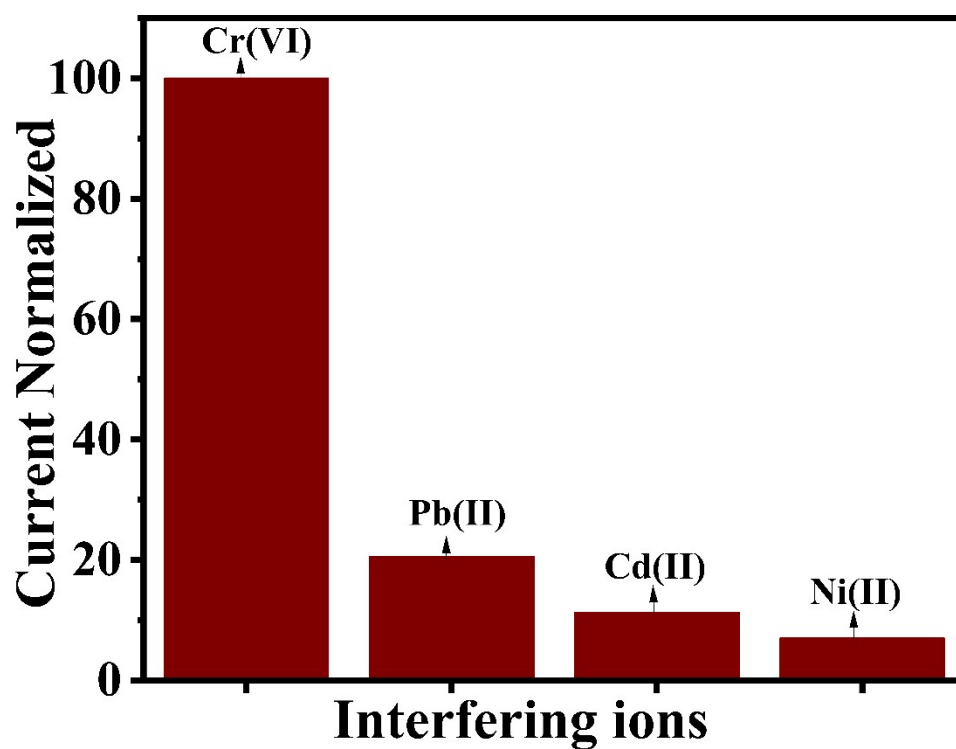
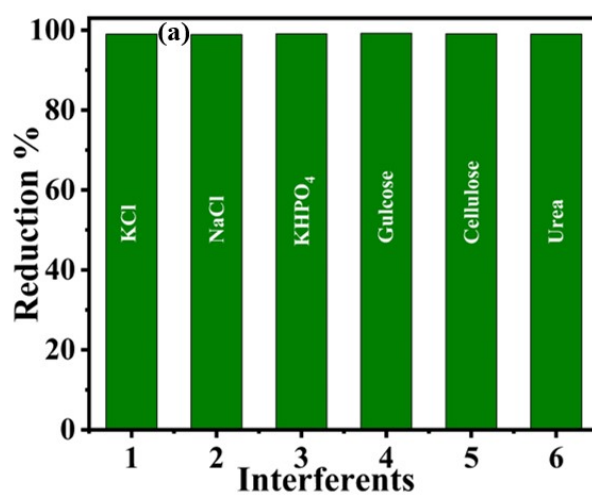


Fig.S8 High-resolution XPS spectra of Cr 2p on h-BN/FeS<sub>2</sub> after reduction reaction





**Fig.S9** represent the electrochemical behaviour of h-BN/FeS<sub>2</sub>/GCE in the presence of various potential interferent ions.



**Fig. S10** (a) Effect of different interfering substances on Cr (VI) reduction