

Supplementary 1: Path length, electron density and Laplacian of bond critical points (BCP) of Cr⁺³-O in the 4-IPC4-Cr⁺³ complex.

Bond	BCP Path length	ρ	$(\nabla^2\rho)$
Cr ⁺³ -O31	1.98	0.0734	0.3613
Cr ⁺³ -O29	2.03	0.0626	0.315
Cr ⁺³ -O27	2.00	0.0702	0.3481
Cr ⁺³ -O25	2.00	0.0707	0.3418

Supplementary 2: Optimization of the membrane composition for fabricated chromium (III)-selective electrode.

*Average and standard deviation for triplet measurements.

Sensor No.	I	PVC	Plasticizer				Lipophilic additive				Nernstian slope* (mV decade ⁻¹)	R ²	Response time (s)
			DOP	DBP	o-NPOE	BA	KTpClPB	NaTFPB	TDATpClPB	NaTPB			
1	0	33.0	—	—	66.5	—	—	—	—	0.5	4.85±0.52	0.98	N/A
2	3.0	33.0	—	—	63.5	—	—	—	—	0.5	13.05±0.37	0.99	16
3	4.0	33.0	—	—	62.5	—	—	—	—	0.5	15.75±0.29	0.99	12
4	5.0	33.0	—	—	61.5	—	—	—	—	0.5	19.45±0.21	0.99	8
5	5.0	33.0	61.5	—	—	—	—	—	—	0.5	18.17±0.52	0.93	14
6	5.0	33.0	—	61.5	—	—	—	—	—	0.5	17.13±0.35	0.90	11
7	5.0	33.0	—	—	—	61.5	—	—	—	0.5	11.94±0.47	0.94	17
8	5.0	33.0	—	—	61.0	—	—	—	—	1.0	21.92±0.46	0.99	11
9	5.0	33.0	—	—	60.5	—	—	—	—	1.5	24.32±0.53	0.97	13
10	5.0	33.0	—	—	61.5	—	0.5	—	—	—	25.50±0.32	0.99	14
11	5.0	33.0	—	—	61.5	—	—	0.5	—	—	27.29±1.16	0.98	14
12	5.0	33.0	—	—	61.5	—	—	—	0.5	—	18.11±0.77	0.88	12

Supplementary 3: Comparison of the selectivity coefficient of fabricated Cr^{3+} -selective electrode in this study with reported chromium electrodes.

Interfering ions (j)	Selectivity coefficient ($\text{Log } K_{\text{Cr},M}^{\text{Pot}}$)								This work
	Ref.1	Ref.2	Ref.3	Ref.4	Ref.5	Ref.6	Ref.7	Ref.8	
Cs^+	-2.10	-	-	-	-	-	-3.79	-	-4.54
Na^+	-0.91	-2.51	-3.70	-3.53	-	-0.76	-3.39	-2.00	-4.13
Li^+	-0.68	-	-	-3.26	-2.96	-0.74	-	-	-4.03
Rb^+	-1.90	-	-	-	-	-	-	-	-3.07
Ag^+	-	-1.00	-	-2.50	-	-2.35	-	-	-3.83
K^+	-0.90	-1.14	-3.20	-3.00	-2.44	-	-3.55	-	-4.29
Zn^{2+}	-1.87	-	-3.10	-3.50	-2.17	-0.65	-3.30	-3.40	-3.35
Ni^{2+}	-2.05	-2.40	-	-3.51	-1.92	-2.49	-3.07	-2.00	-4.01
Ba^{2+}	-2.10	-	-	-	-3.39	-1.05	-3.43	-	-4.06
Cd^{2+}	-2.01	-	-	-3.35	-3.00	-2.17	-3.02	-	-4.16
Co^{2+}	-1.74	-2.70	-	-2.80	-2.17	-	-3.15	-2.77	-3.61
Cu^{2+}	-2.05	-1.80	-2.85	-3.01	-2.64	-1.57	-3.00	-	-3.71
Mn^{2+}	-	-0.58		-3.63	-2.60	-	-	-	-3.51
Pb^{2+}	-1.95	-	-3.00	-3.09	-2.96	-2.85	-3.20	-2.74	-3.81
Mg^{2+}	-2.10	-	-3.45	-3.70	-2.46	-1.62	-	-	-3.51
Ca^{2+}	-1.87	-	-	-2.60	-3.28	-1.86	-3.37	-2.00	-3.91
La^{3+}	-	-	-3.41	-	-	-4.57	-2.60	-2.71	-3.95
Ce^{3+}	-	-	-	-	-	-	-2.72	-3.22	-3.64
Al^{3+}	-3.20	-	-	-	-3.28	-3.15	-2.44	-	-3.44
Nd^{3+}	-	-	-	-	-	-	-	-	-3.30
Fe^{3+}	-3.18	-1.01	-	-	-0.12	-3.65	-	-2.00	-3.85

NOTE: Ref 1: [1], Ref 2: [2], Ref 3: [3], Ref 4: [4], Ref 5: [5], Ref 6: [6], Ref 7: [7], Ref 8: [8].

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