Supporting Information

Geometries and Stabilities of Chromium doped Nitrogen Clusters: Mass Spectrometry and Density Functional Theory Studies

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Table S1. The calculated total energies and lowest frequencies of all ground states and metastable isomers of optimized neutral CrN_n clusters (n = 2-11).

n	Ground state (na)/eV	Frequency (na)/cm^{-1}	Isomer (nb) /eV	Frequency (nb)/cm^{-1}	Isomer (nc) /eV	Frequency (nc)/cm^{-1}
2	-31398.685	64.98	-31397.569	395.23	-31392.378	281.16
3	-32886.998	105.72	-32886.499	56.37	-32885.993	116.62
4	-34378.884	52.60	-34378.248	57.74	-34376.223	89.34
5	-35867.758	40.70	-35867.173	36.76	-35866.713	73.04
6	-37359.281	22.62	-37359.027	59.13	-37358.945	40.56
7	-38847.673	27.32	-38847.646	15.62	-38847.605	46.75
8	-40339.788	17.99	-40339.639	28.08	-40339.513	20.59
9	-41828.048	10.81	-41828.045	12.22	-41827.961	35.28
10	-43320.045	10.42	-43320.023	24.09	-43317.161	23.54
11	-44809.452	25.48	-44809.433	12.73	-44801.661	36.98

Table S2. The calculated total energies and lowest frequencies of all ground states and metastable isomers of optimized cationic CrN_n^+ clusters (n = 2-11).

n	Ground state (na')/eV	Frequency (na')/cm^{-1}	Isomer (nb') /eV	Frequency (nb')/cm^{-1}	Isomer (nc') /eV	Frequency (nc')/cm^{-1}
2	-31392.675	182.77	-31392.246	134.80	-31385.171	192.36
3	-32879.964	99.63	-32879.149	82.29	-32875.991	426.95
4	-34373.823	47.02	-34373.346	43.04	-34372.890	39.09
5	-35861.133	43.81	-35859.853	76.77	-35856.594	206.95
6	-37354.633	30.61	-37354.303	29.60	-37347.551	39.53
7	-38842.137	38.86	-38841.714	21.78	-38838.104	5.13
8	-40335.439	37.18	-40328.400	16.93	-40328.306	37.36
9	-41822.743	24.58	-41813.638	60.54	-41809.886	29.49
10	-43315.958	20.88	-43309.193	16.72	-43309.006	47.63
11	-44803.348	37.79	-44803.333	32.52	-44803.120	29.40

Table S3. The HOMO-LUMO gap values (HLGs) (in eV) of open-shell structure of the low-lying $CrN_n^{0/+}$ cluster (n = 2-11) via the representations of α- (spin-up) and β-orbital (spin-down).

n	CrN_n		CrN_n^+	
	Alpha	Beta	Alpha	Beta
2	5.26	3.58	7.28	12.31
3	5.38	2.77	8.53	8.12
4	5.77	2.77	7.57	10.52
5	5.96	4.23	8.53	8.62
6	5.99	2.77	7.66	11.37
7	4.16	6.57	9.01	9.70
8	6.74	3.22	8.23	13.33
9	4.04	6.91	8.69	9.57
10	6.54	1.41	7.89	12.94
11	5.76	5.14	9.01	9.55

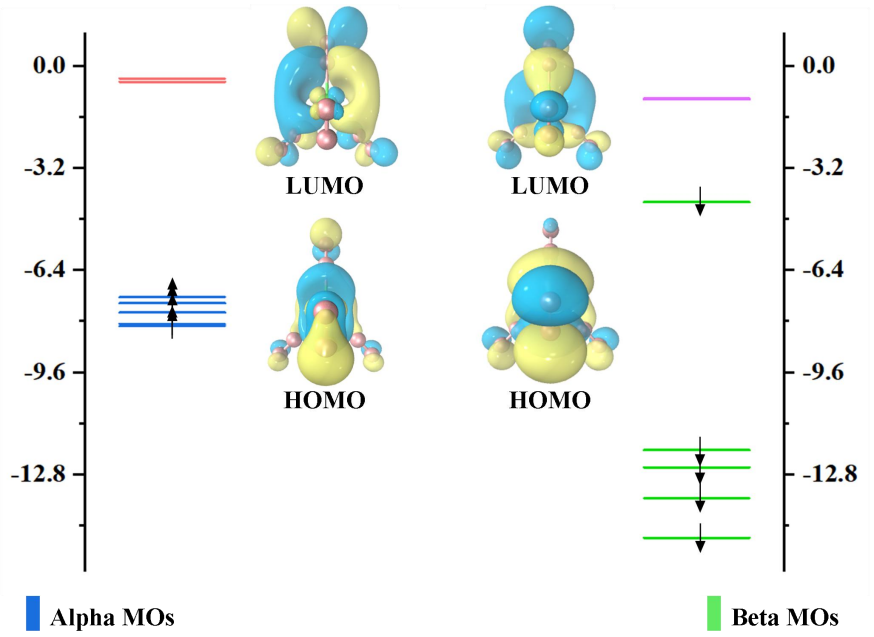

Figure S4. The molecular orbitals of the ground state structure of CrN_8 cluster. The blue and green lines indicate positions of the occupied α and β orbitals, while the red and pink lines indicate the unoccupied α and β orbitals, respectively.

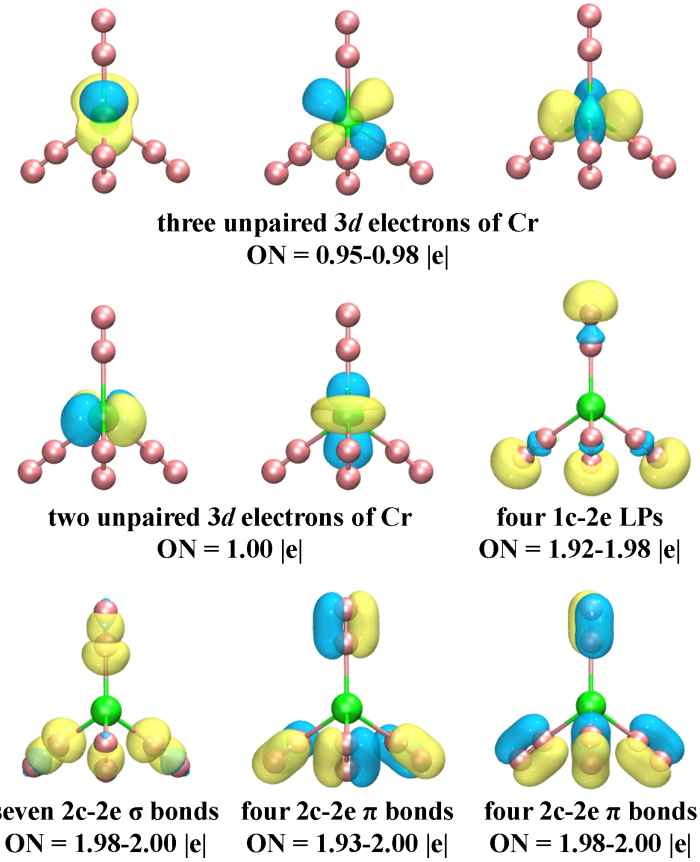

Figure S5. AdNDP analysis of the ground state structure of CrN_8 cluster. ON indicates the number of occupied electrons.