Supporting Information for

Gas-Phase Preparation and the Stability of Superatomic $Nb_{11}O_{15}^-$

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S1. Experimental details

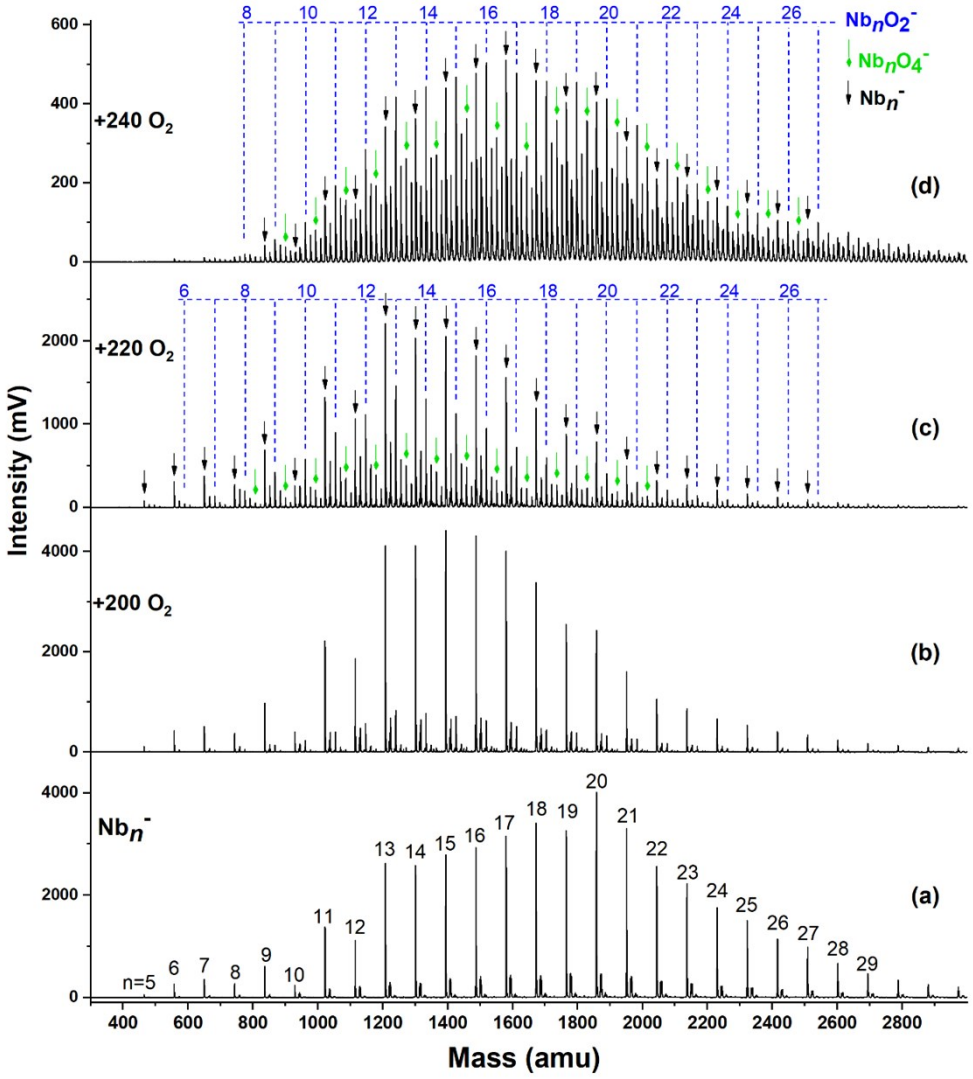

Fig. S1 Mass spectra of the nascent Nb_n^- clusters (a) and in the presence of different flow rate of oxygen reactant (1% O_2 in He) injected by a 10Hz pulse valve with the on-time per period at 200 μs (b), 220 μs (c), and 240 μs(d) respectively. The peaks marked with black arrows refer to the pure Nb_n^- clusters, while the blue and green arrows correspond to the $Nb_nO_2^-$ and $Nb_nO_4^-$ products, respectively.

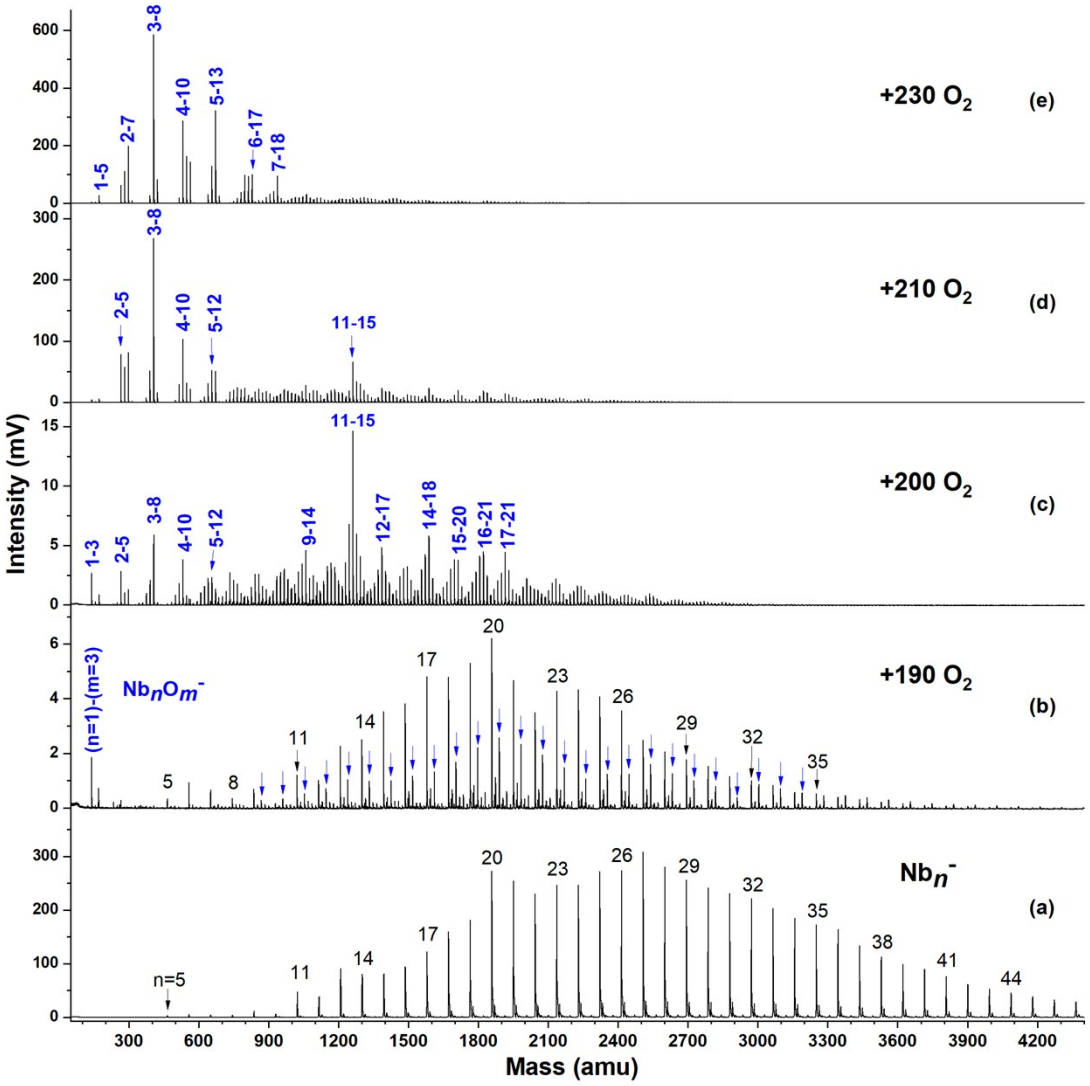

Fig. S2 Mass spectra of the nascent Nb_n^- clusters (a) and in the presence of different flow rate of oxygen reactant (20 % O_2 in He) injected by a 10 Hz pulse valve with the on-time per period at (b) 190 μs, (c) 200 μs, (d) 210 μs, (e) 230 μs respectively. The blue arrows referring to the $Nb_nO_2^-$ clusters.

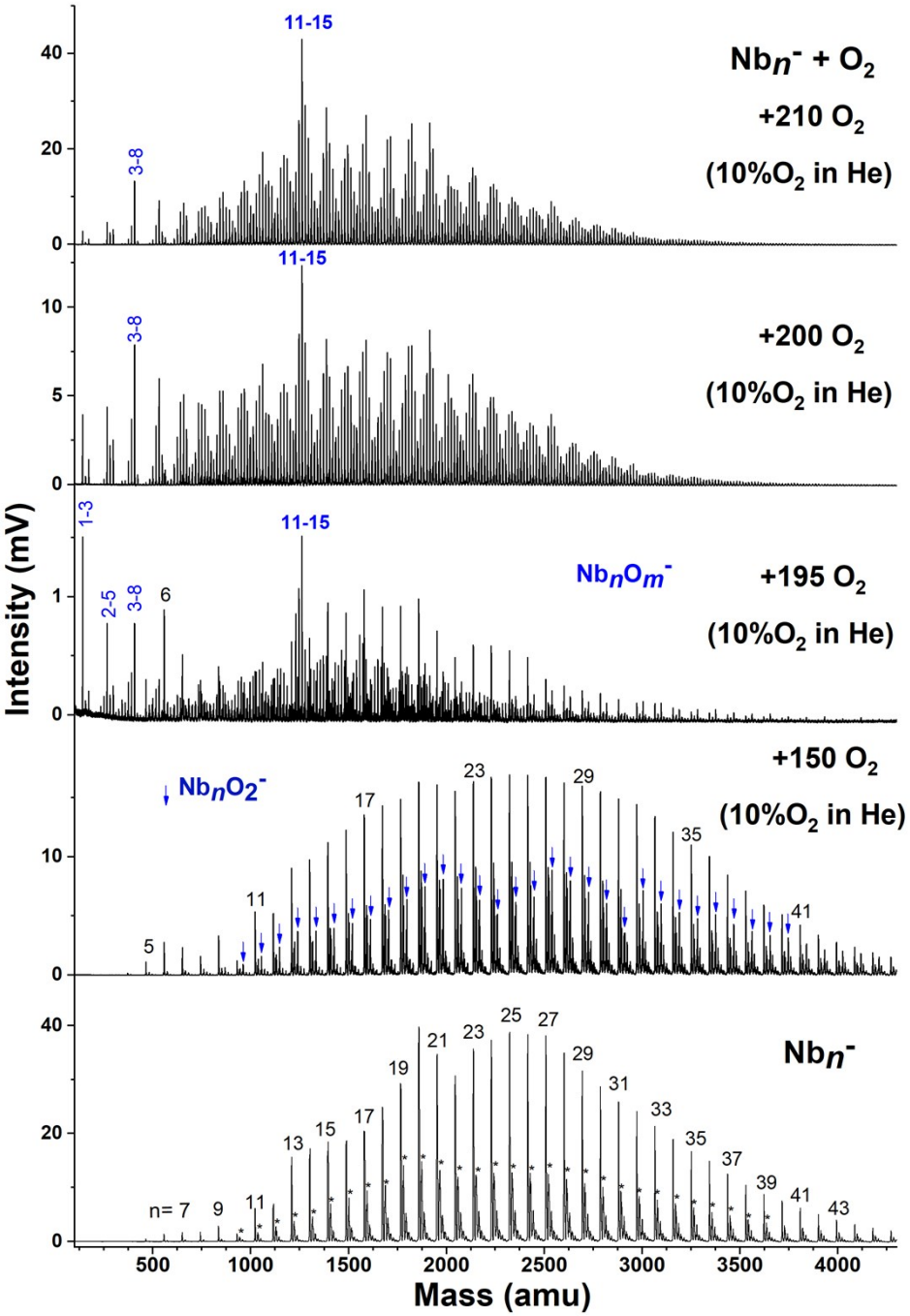

Fig. S3 Repeated experiments showing the mass spectra of Nb_n^- clusters (a) and the products with 10% O_2 in He, injected by a 10 Hz pulse valve with the on-time per period at (b) 150 μs, (c) 195 μs, (d) 200 μs, (e) 210 μs respectively, with the blue arrows referring to the $Nb_nO_2^-$ clusters.

S2. Reaction rate estimation

Considering that the small concentration of oxygen react with the niobium clusters to produce oxygen-addition products, we have estimated the reaction rate constants by assuming the initial reactions within a pseudo-first-order reaction, for which the rate constants k can be estimated by the following equation,[1-4]

$$\ln(I_A/I_0) = -k \cdot p \cdot \Delta t/(k_B \cdot T) \quad (1)$$

in which the variable I_A stands for the parent ion intensity at a certain O_2 gas pressure, and I_0 refers to the total signal intensity including both the reactant cluster ion intensity and the product ion intensity. The p refers to the effective pressure of the reactant gas calculated from the molecular density of the reactant gas. The k_B is the Boltzmann constant, T the temperature of the reactant gas, and Δt the effective reaction time in the flow tube reactor (~60μs)[5]. The effective pressure p is calculated with the ideal gas law $P = \rho \cdot k_B \cdot T$. ρ refers to the molecular density of the reactant gas, and is determined by $\rho = N/(t \cdot U \cdot S)$. *N* is the molecule number of reaction gas per pulse. t is the time sequence difference between the carrier gas. S is the cross-sectional areas defined by the inner diameters of the fast-flow reactor. U is the flowing velocity of cluster beam in the fast-flow reactor. The value of ρ is obtained by experimental calibration, and the details have been described elsewhere.[6, 7]

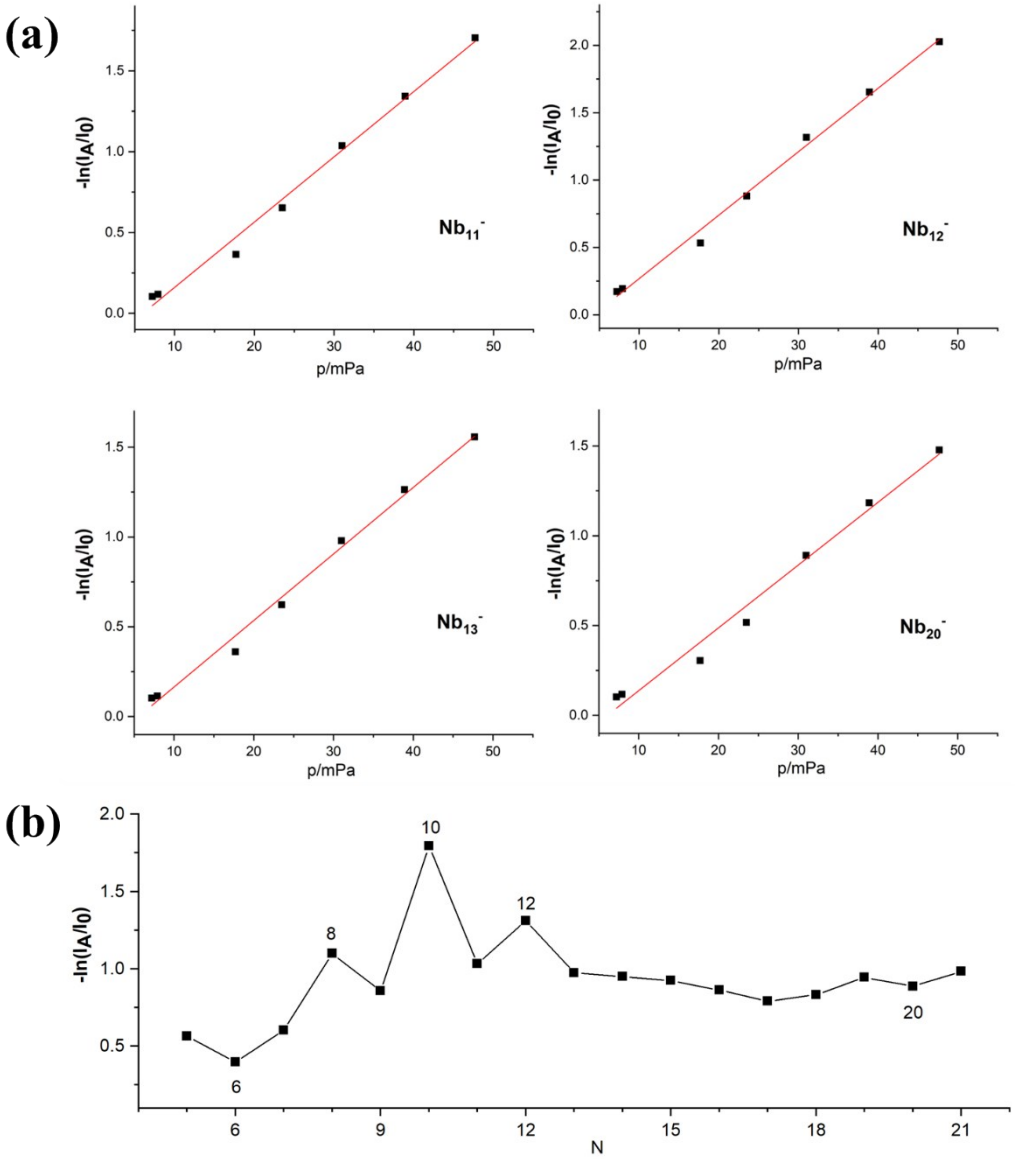

Fig. S4 (a) Linear fitting of $-\ln(I_A/I_0)$ vs. partial pressures of O_2 for $Nb_{11\text{-}13}^-$ and Nb_{20}^-; **(b)** Experimentally determined $-\ln(I_A/I_0)$ for the reactions between Nb_n^- (n = 5-21) and O_2 with 1% O_2 in He injection by a 10Hz pulse valve with the on-time per period at 220μs. A good linear correlation between $-\ln(I_A/I_0)$ and the partial pressures of O_2 is obtained as is shown in (a) for the randomly drawing $Nb_{11\text{-}13}^-$ and Nb_{20}^- clusters, implying the incipient reactions between the Nb_n^- clusters and O_2 in the flow tube follow a pseudo-first-order mechanism. For Nb_n^-, n= 7-13, the pseudo-first-order rate constants (in proportion to $-\ln(I_A/I_0)$) for Nb_n^- with O_2 follow the even/odd effect, as shown in (b).

S3. Structure determination and energetics

S3.1 Nb_n^- Clusters

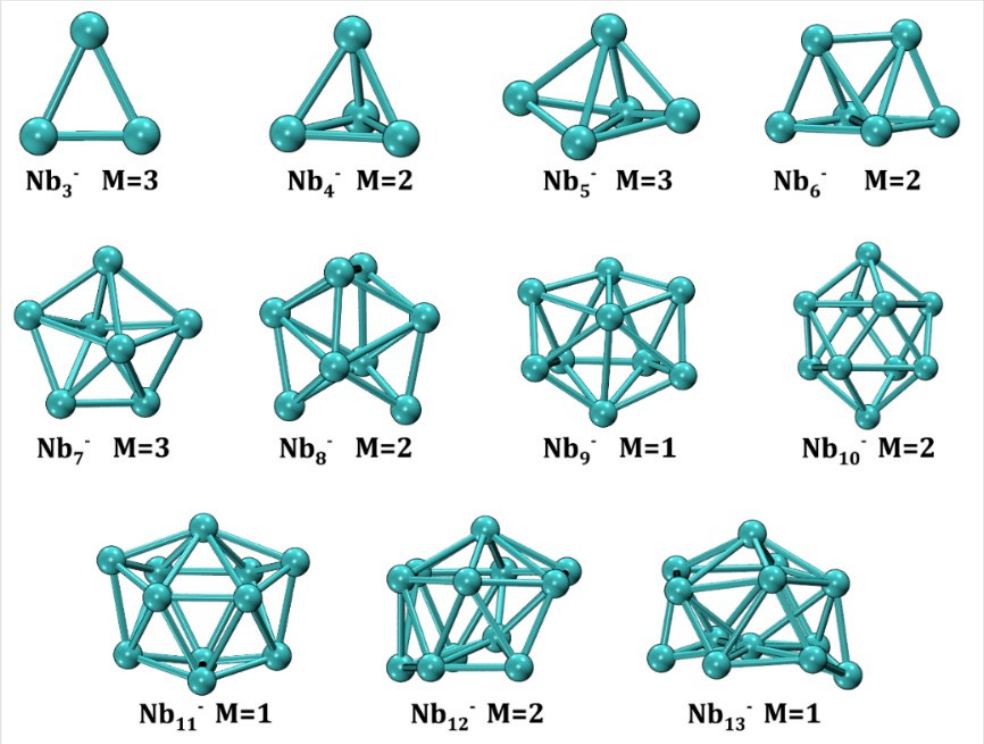

Fig. S5 The optimized structures of anionic Nb_n^- (n=3-13) at B3LYP/def2-TZVP level. M indicates spin multiplicity.

Table S1. VDEs and HOMO-LUMO gaps of the Nb_n^- clusters from Kietzmann work.[8]

n	5	6	7	8	9	10	11	12	13
VDEs (eV)	1.519	1.577	1.649	1.458	1.649	1.456	1.689	1.624	1.700
Gaps (eV)	------	0.231	------	0.704	0.001	0.503	------	0.201	0.002

S3.2 $Nb_nO_m^-$ Clusters

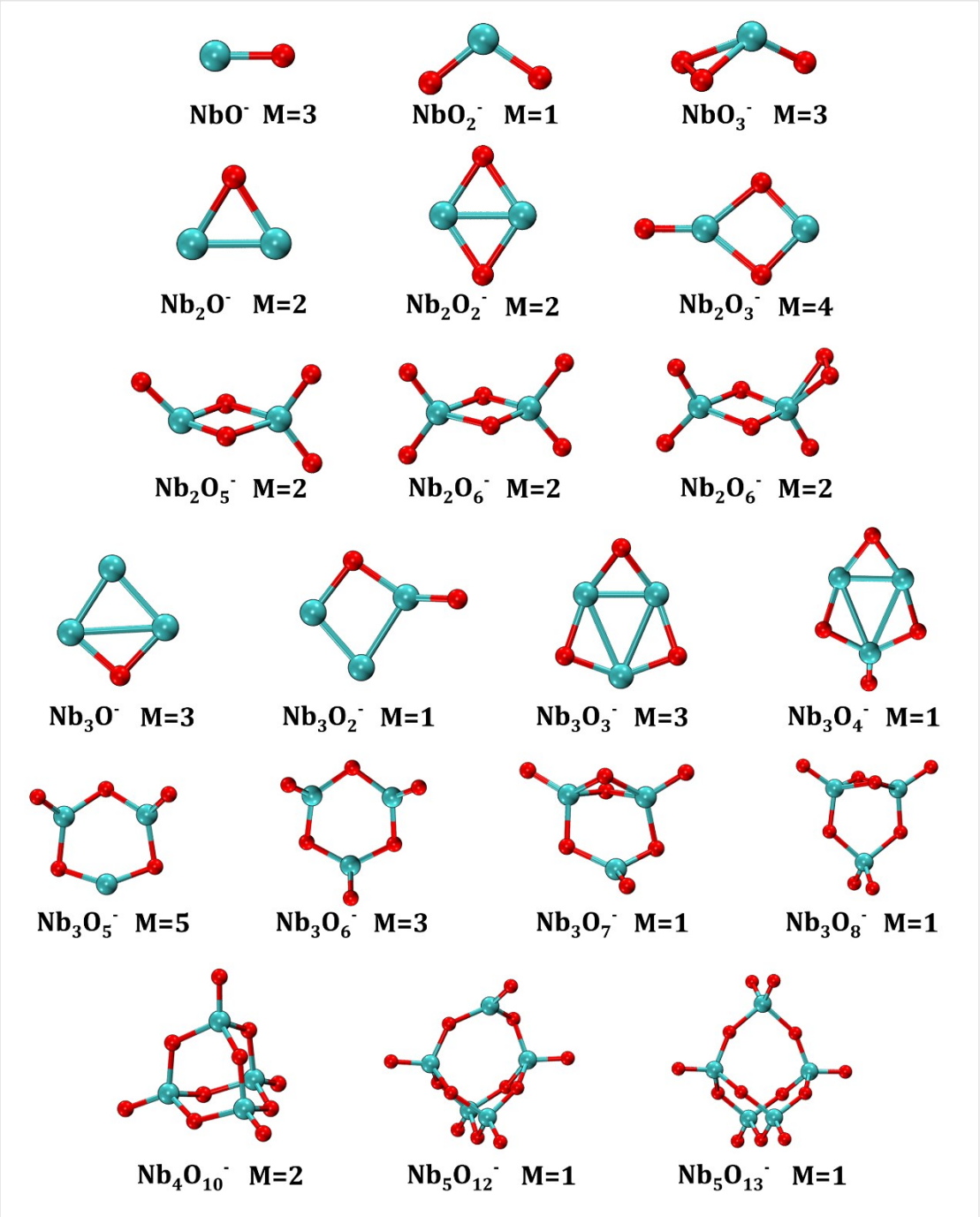

Fig. S6 The optimized structures of anionic $Nb_nO_m^-$ at B3LYP/def2-TZVP level. M indicates spin multiplicity.

Table S2 The HOMO-LUMO gaps and electron detachment energies of the $Nb_nO_m^-$ clusters calculated at B3LYP/def2-TZVP level of theory.

	Spin multiplicity	α gap (eV)	β gap (eV)	VDE (eV)
$Nb_1O_1^-$	3	2.56	2.51	1.79
$Nb_1O_2^-$	1	2.23	-	1.72
$Nb_1O_3^-$	3	2.51	3.95	2.00
$Nb_2O_1^-$	2	0.48	1.66	0.39
$Nb_2O_2^-$	2	1.96	2.2	1.09
$Nb_2O_3^-$	4	2.05	2.38	1.79
$Nb_2O_5^-$	2	3.05	4.35	3.76
$Nb_2O_6^-$	2	4.71	1.35	5.49
$Nb_2O_7^-$	2	4.56	2.21	5.41
Nb_3O^-	3	1.14	1.9	1.75
$Nb_3O_2^-$	1	1.48	-	1.76
$Nb_3O_3^-$	3	1.66	2.08	1.62
$Nb_3O_4^-$	1	1.84	-	2.05
$Nb_3O_5^-$	5	2.42	3.21	2.5753
$Nb_3O_6^-$	3	2.47	3.19	3.08
$Nb_3O_7^-$	1	2.55	-	3.49
$Nb_3O_8^-$	1	4.03	-	5.80
$Nb_4O_{10}^-$	2	1.52	5.55	3.12
$Nb_5O_{12}^-$	1	2.52	-	4.33
$Nb_5O_{13}^-$	1	3.61	-	6.18
$Nb_{11}O_{15}^-$	1	1.48	-	3.09 (ADE=2.77eV)

S3.3 The $Nb_{11}O_{15}^-$

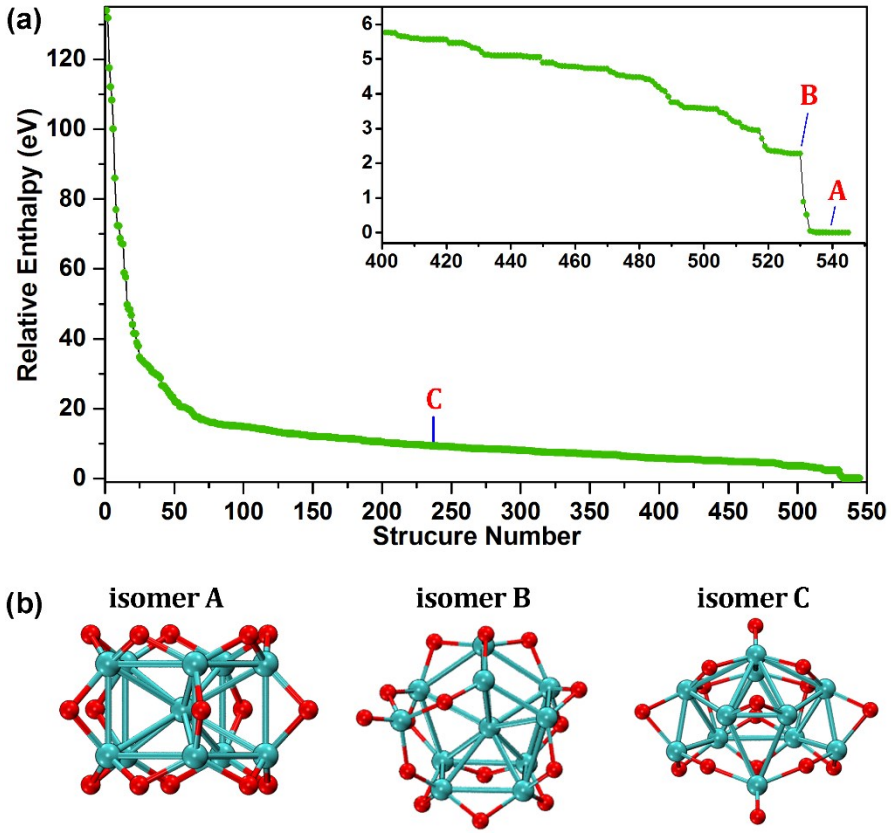

Fig. S7 (a) The energy evolutionary simulation of the global minimum structures for neutral $Nb_{11}O_{15}$ based on USPEX combined with VASP. **(b)** isomer structures with relative lower energies labeled in (a).

Table S3. Relative Energy (ZPVE, eV) of $Nb_{11}O_{15}^-$ isomers.

$Nb_{11}O_{15}^-$	**spin multiplicity**	**B3LYP/def2TZVP ΔE (eV)**	**BPW91/def2TZVP ΔE (eV)**
A	1	0.00	0.00
	3	0.17	0.12
	5	0.16	\
B	1	1.88	2.08
C	1	9.45	7.67

S4. Wiberg bond order

Table S4 Natural atomic charges (q/|e|), electronic configurations, and Wiberg bond orders of the central Nb atom, the 10 Nb-ligands and 15 O-bridges in $Nb_{11}O_{15}^-$, calculated at B3LYP/def2-TZVP level of theory using NBO6.0 method.

	Atoms	Atomic charges q	Electronic Configurations	Wiberg bond order indexes
D_{5h} $Nb_{11}O_{15}^-$ ($^1A_1'$)	Nb_1	−0.804	$[Kr]5s^{0.87}4d^{4.87}5p^{0.05}5d^{0.04}$	6.33
	$Nb_{2\text{-}11}$	+1.368 ~ +1.367	$[Kr]5s^{0.36}4d^{3.23}5p^{0.03}4f^{0.01}5d^{0.05}$	3.77
	Nb_1-$Nb_{2\text{-}11}$	------	------	0.60
	$O_{1\text{-}10}$	−0.920	$[He]2s^{1.80}2p^{5.10}3s^{0.01}3p^{0.01}3d^{0.01}$	1.28
	$O_{11\text{-}15}$	−0.934	$[He]2s^{1.79}2p^{5.11}3s^{0.01}3p^{0.01}3d^{0.01}$	1.29

S5. Reaction channel and thermodynamics

Table S5. Proposed reaction channels, calculated at the B3LYP/def2-TZVP level of theory.

Proposed reaction channels	**Examples**	**ΔH (eV)**
(1) $Nb_n^- \xrightarrow{O_2} Nb_nO_2^- \xrightarrow{O_2} Nb_nO_4^-$	$Nb_3^- + O_2 \rightarrow Nb_3O_2^-$	-9.64
	$Nb_3O_2^- + O_2 \rightarrow Nb_3O_4^-$	-10.02
(2) $Nb_n^- + O_2 \rightarrow Nb_nO^- + O^*$	$Nb_3^- + O_2 \rightarrow Nb_3O^- + O^*$	-2.68
(3) $Nb_n^- + m\ O_2 \rightarrow Nb_{n-1}O_{2m-1}^- + NbO$	$Nb_3^- + O_2 \rightarrow Nb_2O^- + NbO$	-4.64
(4) $Nb_n^- + m\ O_2 \rightarrow Nb_{n-1}O_{2m-2}^- + NbO_2$	$Nb_3^- + 2\ O_2 \rightarrow Nb_2O_2^- + NbO_2$	-11.78
(5) $Nb_n^- + m\ O_2 \rightarrow Nb_{n-2}O_{2m-5}^- + Nb_2O_5$	$Nb_3^- + 3\ O_2 \rightarrow NbO^- + Nb_2O_5$	-22.75
(6) $Nb_n^- + O_2 \rightarrow Nb_{n-1}O^- + NbO$	$Nb_3^- + O_2 \rightarrow Nb_2O^- + NbO$	-4.64
(7) $Nb_{n-1}O^- + O_2 \rightarrow Nb_{n-1}O_3^-$	$Nb_2O^- + O_2 \rightarrow Nb_2O_3^-$	-9.46
(8) $Nb_{n-1}O_3^- + O_2 \rightarrow Nb_{n-1}O_5^-$	$Nb_2O_3^- + O_2 \rightarrow Nb_2O_5^-$	-10.29
(9) $Nb_n^- + m\ O_2 \rightarrow Nb_{n-1}O_{2m-1} + NbO_1^-$	$Nb_3^- + O_2 \rightarrow Nb_2O + NbO^-$	-6.08
(10) $Nb_n^- + m\ O_2 \rightarrow Nb_{n-1}O_{2m-3} + NbO_3^-$	$Nb_3^- + 3\ O_2 \rightarrow Nb_2O_3 + NbO_3^-$	-18.64
(11) $NbO_3^- + NbO_2 \rightarrow Nb_2O_5^-$	$NbO_3^- + NbO_2 \rightarrow Nb_2O_5^-$	-11.58
(12) $NbO_3^- + Nb_2O_5 \rightarrow Nb_3O_8^-$	$NbO_3^- + Nb_2O_5 \rightarrow Nb_3O_8^-$	-11.26
(13) $Nb_2O_5^- + Nb_2O_5 \rightarrow Nb_4O_{10}^-$	$Nb_2O_5^- + Nb_2O_5 \rightarrow Nb_4O_{10}^-$	-7.79
(14) $Nb_3O_8^- + Nb_2O_5 \rightarrow Nb_5O_{13}^-$	$Nb_3O_8^- + Nb_2O_5 \rightarrow Nb_5O_{13}^-$	-6.69
(15) $Nb_n^- + m\ O_2 \rightarrow Nb_{11}O_{15}^- + x\ NbO + y\ NbO_2 + z\ Nb_2O_5$ （n=11+x+y+2z; 2m=15+x+2y+5z）	$Nb_{12}^- + 8\ O_2 \rightarrow Nb_{11}O_{15}^- + NbO$	**-77.64**
	$Nb_{13}^- + 9\ O_2 \rightarrow Nb_{11}O_{15}^- + NbO + NbO_2$	**-79.70**
	$Nb_{13}^- + 10\ O_2 \rightarrow Nb_{11}O_{15}^- + Nb_2O_5$	**-93.94**

S6. Molecular dynamics simulation

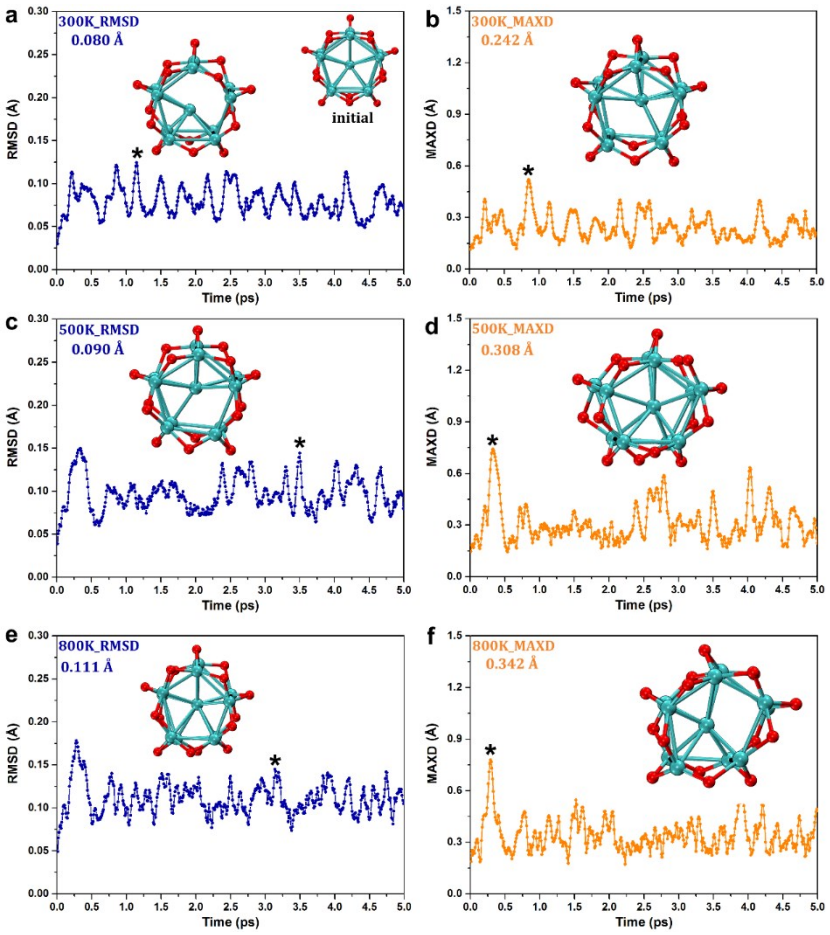

Fig. S8 Born-Oppenheimer molecular dynamics simulations of *D*5h $Nb_{11}O_{15}^-$ at 300K, 500K, 800K for 5 ps, with the average root-mean-square-deviation (RMSD) values and maximum bond length deviation (MAXD) values indicated in Å.

S7. Density of states and molecular orbitals

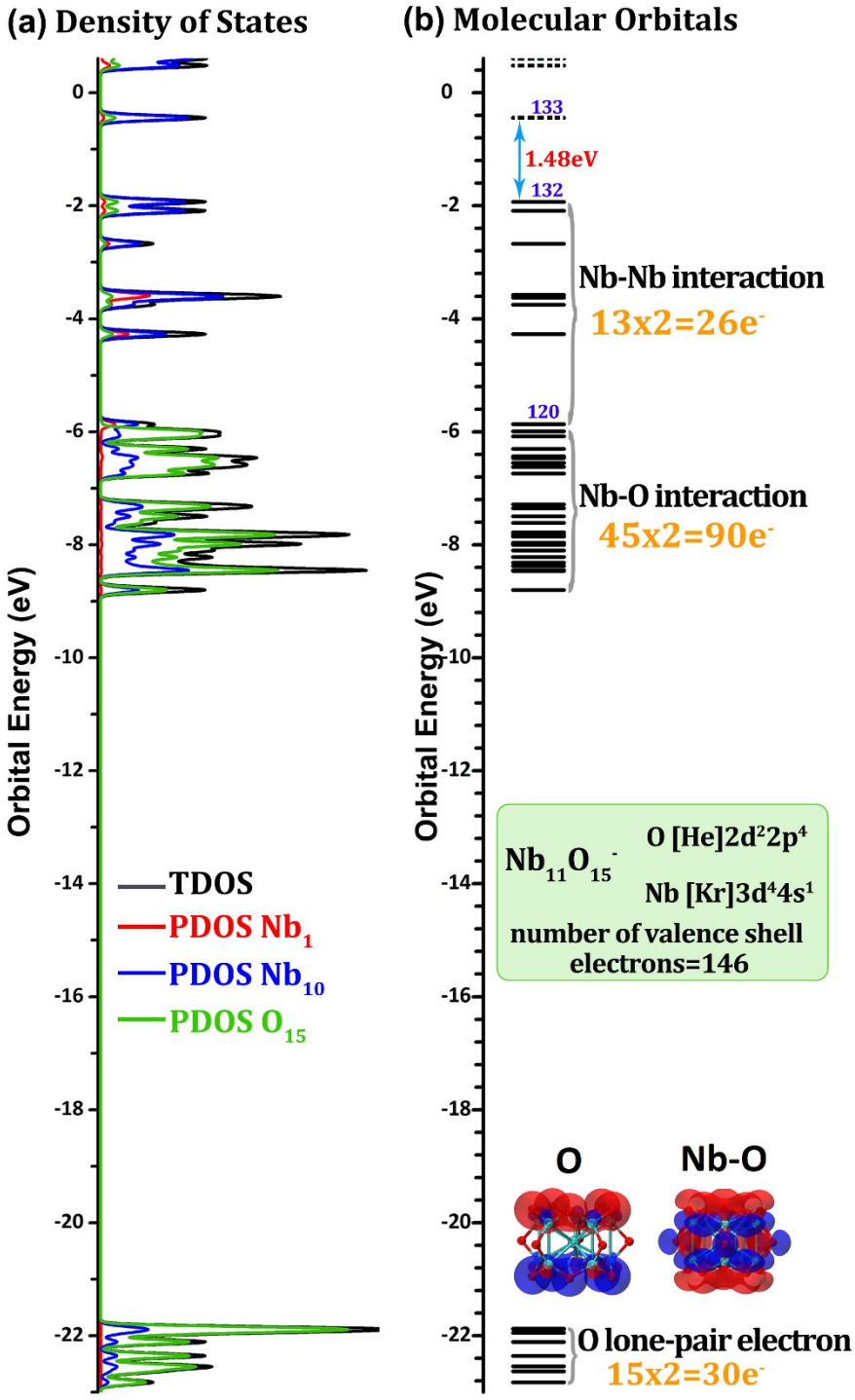

Fig. S9 Total and partial density of states (DOS) of the $Nb_{11}O_{15}^-$ cluster by dividing the total DOS of the cluster into contributions of Nb_1 (in red), Nb_{10} (in blue), and O_{15} (in green). (b) Frontier canonical molecular orbitals (CMOs) of $Nb_{11}O_{15}^-$, with their superatomic features (including MOs from 120 to 132) (S, P, D and F) indicated.

S8. Energy decomposition analysis

Table S6 Energy decomposition analysis (EDA)[9] results for $Nb_{11}O_{15}^-$ at different theoretical level taking $Nb_{10}O_{15}$ and Nb^- as interacting fragments. Energy values are given in kcal/mol.

Theoretical Level	Total Bonding Energy ΔE_{tot}	Electrostatic Interaction ΔE_{elstat}	Pauli Repulsion ΔE_{pauli}	Orbital Interactions ΔE_{orb}
B3LYP/TZP	-451.12	-1180.70	1537.94	**-808.35**
PBE0/TZP	-509.20	-1218.00	1545.93	**-837.12**
PBE/TZP	-419.78	-1167.82	1473.11	**-725.06**
BP86/TZP	-409.21	-1149.68	1465.59	**-725.10**

$$\Delta E_{tot} = \Delta E_{pauli} + \Delta E_{elstat} + \Delta E_{orb}$$

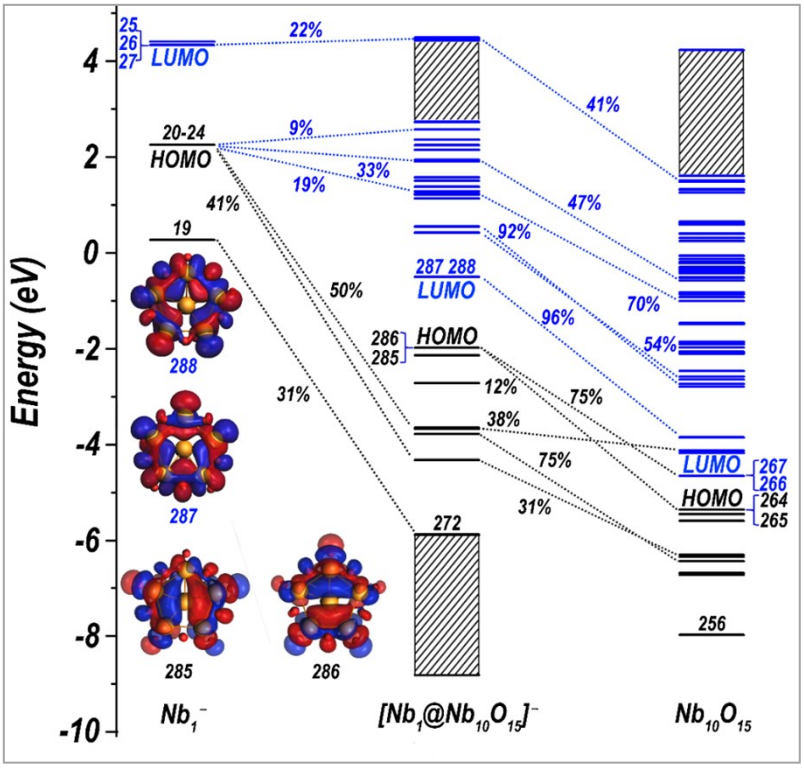

Fig. S10 Kohn-Sham energy-level correlation diagram of $[Nb@Nb_{10}O_{15}]^-$ cluster at the SR-ZORA B3LYP/TZP level of theory. The occupied and virtual orbitals are marked in black and blue, respectively.

References

1. B. Yin, Q. Du, L. Geng, H. Zhang, Z. Luo, S. Zhou and J. Zhao, *J. Phys. Chem. Lett.*, 2020, **11**, 5807-5814.
2. B. Yin, Q. Du, L. Geng, H. Zhang, Z. Luo, S. Zhou and J. Zhao, *CCS Chemistry*, 2021, **3**, 1–13.
3. H. Zhang, H. Wu, L. Geng, Y. Jia, M. Yang and Z. Luo, *Phys. Chem. Chem. Phys.*, 2019, **21**, 11234-11241.
4. H. Zhang, H. Wu, Y. Jia, B. Yin, L. Geng, Z. Luo and K. Hansen, *Commun. Chem.*, 2020, **3**, 148.
5. B. Q. Yin, Q. Y. Du, L. J. Geng, H. Y. Zhang, Z. X. Luo, S. Zhou and J. J. Zhao, *J. Phys. Chem. Lett.*, 2020, **11**, 5807-5814.
6. H. Y. Zhang, H. M. Wu, L. J. Geng, Y. H. Jia, M. Z. Yang and Z. X. Luo, *Phys. Chem. Chem. Phys.*, 2019, **21**, 11234-11241.
7. H. Y. Zhang, H. M. Wu, Y. H. Jia, L. J. Geng, Z. X. Luo, H. B. Fu and J. N. Yao, *Rev. Sci. Instrum.*, 2019, **90**, 073101.
8. H. Kietzmann, J. Morenzin, P. S. Bechthold, G. Gantefor and W. Eberhardt, *J. Chem. Phys.*, 1998, **109**, 2275-2278.
9. M. v. Hopffgarten and G. Frenking, *WIREs Comput. Mol. Sci.*, 2012, **2**, 43-62.

Appendix

The coordinates of all the optimized niobium oxides in this study

NbO-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	-1.434438
2	41	0	0.000000	0.000000	0.279890

NbO2-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	1.387342	-0.750092
2	8	0	0.000000	-1.387342	-0.750092
3	41	0	0.000000	0.000000	0.292719

NbO3-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.642685	-0.790160	0.000604
2	8	0	1.482720	-0.313648	0.735151
3	8	0	1.482582	-0.314864	-0.734729
4	41	0	-0.258072	0.276814	-0.000200

Nb2O-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	-0.296973	1.009071	0.000000
2	41	0	0.000000	-1.051800	0.000000
3	8	0	1.521988	0.218983	0.000000

Nb2O2-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.001266	-1.647231	0.000000
2	8	0	0.001262	1.647230	0.000000
3	41	0	1.092418	-0.000372	0.000000
4	41	0	-1.092418	0.000372	0.000000

Nb2O3-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.391527	-1.327603	-0.000422
2	8	0	0.391495	1.327606	-0.000422
3	8	0	-2.989036	0.000019	0.001382
4	41	0	1.665764	0.000005	0.000255
5	41	0	-1.235322	-0.000009	-0.000360

Nb2O5-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	0.076286	1.336874	0.000000
2	41	0	0.088917	-1.603449	0.000000
3	8	0	0.088917	-0.249305	1.315106
4	8	0	0.088917	-0.249305	-1.315106
5	8	0	1.523448	2.328465	0.000000
6	8	0	-1.364621	2.335291	0.000000
7	8	0	-1.183322	-2.798948	0.000000

Nb2O6-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	-0.697351	1.273863	0.000000
2	41	0	0.709111	-1.332367	0.000000
3	8	0	-2.440643	1.530686	0.000000
4	8	0	2.455792	-1.483550	0.000000
5	8	0	-0.057713	-2.908282	0.000000
6	8	0	-0.057713	0.062083	1.301775
7	8	0	0.097721	3.036816	0.000000
8	8	0	-0.057713	0.062083	-1.301775

Nb2O7-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	0.801404	1.036252	0.000000
2	41	0	-0.811463	-1.453840	0.000000
3	8	0	2.534833	1.030556	0.000000
4	8	0	0.067223	-0.131737	1.293674
5	8	0	0.067223	-0.131737	-1.293674
6	8	0	-0.186333	-3.091991	0.000000
7	8	0	0.067223	2.957928	0.665087
8	8	0	0.067223	2.957928	-0.665087
9	8	0	-2.565844	-1.450807	0.000000

Nb3O-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	-1.290608	-0.626685	0.000103
2	41	0	1.448752	-0.324927	0.000097
3	41	0	-0.200548	1.303926	-0.000085
4	8	0	0.217324	-1.805608	-0.000587

Nb3O2-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	1.367036	0.253062	-0.182797
2	41	0	-1.392582	0.735720	0.090967
3	41	0	-0.577171	-1.289928	-0.025236
4	8	0	0.233936	1.809984	-0.054316
5	8	0	2.854992	-0.266612	0.654284

Nb3O3-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	-0.842395	1.112192	-0.093483
2	41	0	1.727993	-0.000005	0.001525
3	41	0	-0.842405	-1.112185	-0.093473
4	8	0	1.076446	1.775402	0.208043
5	8	0	-2.374246	0.000000	0.534279
6	8	0	1.076433	-1.775412	0.208010

Nb3O4-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	1.006279	-1.128297	-0.124377
2	41	0	-1.638743	-0.004609	0.196046

3	41	0	0.992732	1.132169	-0.127534
4	8	0	-0.807790	-1.692559	0.556746
5	8	0	2.564492	0.012247	0.282968
6	8	0	-0.820311	1.685499	0.571159
7	8	0	-2.782765	-0.001410	-1.124562

Nb3O5-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	-1.542645	-0.703268	-0.152099
2	41	0	0.000089	1.841439	0.138877
3	41	0	1.542569	-0.703376	-0.152100
4	8	0	-1.794425	1.246124	-0.215132
5	8	0	2.440497	-1.537876	1.074847
6	8	0	-2.440624	-1.537663	1.074886
7	8	0	1.794567	1.245987	-0.215091
8	8	0	-0.000079	-1.644900	-0.872239

Nb3O6-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	1.725586	-0.465870	-0.113112
2	41	0	-0.459104	1.725923	-0.113520
3	41	0	-1.265626	-1.258934	-0.112185
4	8	0	2.802040	-0.755694	1.212426
5	8	0	0.499548	-1.884018	-0.633041
6	8	0	-0.746584	2.794229	1.219270
7	8	0	1.381334	1.376423	-0.632598
8	8	0	-1.879953	0.507614	-0.641237
9	8	0	-2.060772	-2.044288	1.211617

Nb3O7-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	0.233097	1.504977	-0.001023

2	41	0	1.585563	-1.073652	-0.164159
3	41	0	-1.662729	-0.592878	0.024783
4	8	0	1.768026	0.695931	-0.907056
5	8	0	-1.043266	0.640436	1.334763
6	8	0	-0.237047	-1.886243	-0.146828
7	8	0	2.637084	-1.428531	1.160326
8	8	0	-3.324359	-1.130777	0.076850
9	8	0	-1.167624	0.785512	-1.242731
10	8	0	0.568037	3.151631	0.444221

Nb3O8-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	1.099342	1.420476	0.000126
2	41	0	-2.073526	-0.000034	0.000049
3	41	0	1.098860	-1.420652	-0.000054
4	8	0	-0.761695	1.592942	0.000578
5	8	0	1.469019	-0.000244	1.295914
6	8	0	-0.762122	-1.593956	0.000318
7	8	0	-3.089258	0.001434	1.417498
8	8	0	2.060954	-2.869210	0.000391
9	8	0	-3.087123	0.000668	-1.418956
10	8	0	2.061743	2.869063	-0.000306
11	8	0	1.469515	0.000381	-1.296058

Nb4O10-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.180630	-0.044536	-0.001851
2	8	0	0.044994	2.179647	0.000689
3	8	0	-2.180700	0.044865	0.002798
4	8	0	0.001985	-0.001118	2.067102
5	8	0	-0.002583	0.001080	-2.066992
6	8	0	-2.227114	-2.134860	-2.248958
7	8	0	-0.044580	-2.179353	-0.001389
8	8	0	2.222386	2.136365	-2.252081
9	8	0	-2.132782	2.224194	2.253595
10	8	0	2.137666	-2.226343	2.247077

11	41	0	1.243062	1.194159	-1.179321
12	41	0	1.195491	-1.244397	1.176669
13	41	0	-1.245765	-1.193176	-1.177574
14	41	0	-1.192769	1.243426	1.180228

Nb5O12-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.026653	-1.152603	1.509259
2	8	0	2.551381	-1.060388	-1.078434
3	8	0	-1.077281	1.057376	-1.557965
4	8	0	-1.119400	1.652234	1.394440
5	8	0	-0.339418	-1.921436	-1.304127
6	8	0	-2.841602	-1.137148	-2.806446
7	8	0	-2.673720	-0.753785	0.241877
8	8	0	1.796644	-3.330051	0.606677
9	8	0	1.552940	2.100624	-0.229441
10	8	0	-2.333689	-0.450369	3.319355
11	8	0	-0.778941	3.913450	-0.584168
12	8	0	4.015675	0.545631	1.077459
13	41	0	2.836616	0.593954	-0.178619
14	41	0	1.149867	-1.846238	0.029174
15	41	0	-1.606291	-0.188950	1.774542
16	41	0	-1.803582	-0.737881	-1.486690
17	41	0	-0.328013	2.283790	-0.253233

Nb5O13-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.792063	1.539226	1.512097
2	8	0	-1.923182	1.576515	-0.000123
3	8	0	0.792220	-1.539210	-1.512078
4	8	0	0.792032	-1.539264	1.512049
5	8	0	0.792250	1.539268	-1.512028
6	8	0	2.904624	0.000031	-3.081236
7	8	0	2.899568	-0.000015	0.000148
8	8	0	-0.234100	3.999248	-0.000005
9	8	0	-1.923217	-1.576530	-0.000174

10	8	0	2.904227	-0.000061	3.081535
11	8	0	-0.234114	-3.999242	-0.000127
12	8	0	-4.232023	-0.000004	1.418557
13	8	0	-4.232259	0.000041	-1.418543
14	41	0	-0.215964	2.277783	-0.000020
15	41	0	1.915069	0.000019	-1.672631
16	41	0	-0.215989	-2.277777	-0.000089
17	41	0	-3.221985	0.000007	-0.000077
18	41	0	1.914852	-0.000032	1.672803

Nb11O15-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	41	0	-2.437424	0.791967	1.406213
2	41	0	0.000000	2.562860	1.406213
3	41	0	-1.506411	-2.073397	1.406213
4	41	0	2.437424	0.791967	1.406213
5	41	0	0.000000	0.000000	0.000000
6	41	0	1.506411	-2.073397	-1.406213
7	41	0	0.000000	2.562860	-1.406213
8	41	0	2.437424	0.791967	-1.406213
9	41	0	-1.506411	-2.073397	-1.406213
10	41	0	-2.437424	0.791967	-1.406213
11	41	0	1.506411	-2.073397	1.406213
12	8	0	0.000000	3.893376	0.000000
13	8	0	-3.702820	1.203119	0.000000
14	8	0	-1.696165	2.334571	2.300530
15	8	0	-2.744452	-0.891727	2.300530
16	8	0	1.696165	2.334571	2.300530
17	8	0	2.744452	-0.891727	2.300530
18	8	0	3.702820	1.203119	0.000000
19	8	0	0.000000	-2.885688	2.300530
20	8	0	2.744452	-0.891727	-2.300530
21	8	0	-2.288469	-3.149807	0.000000
22	8	0	1.696165	2.334571	-2.300530
23	8	0	-2.744452	-0.891727	-2.300530
24	8	0	2.288469	-3.149807	0.000000
25	8	0	-1.696165	2.334571	-2.300530
26	8	0	0.000000	-2.885688	-2.300530