Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information

Anion Ordering and Vacancy Defects in Niobium Perovskite Oxynitrides

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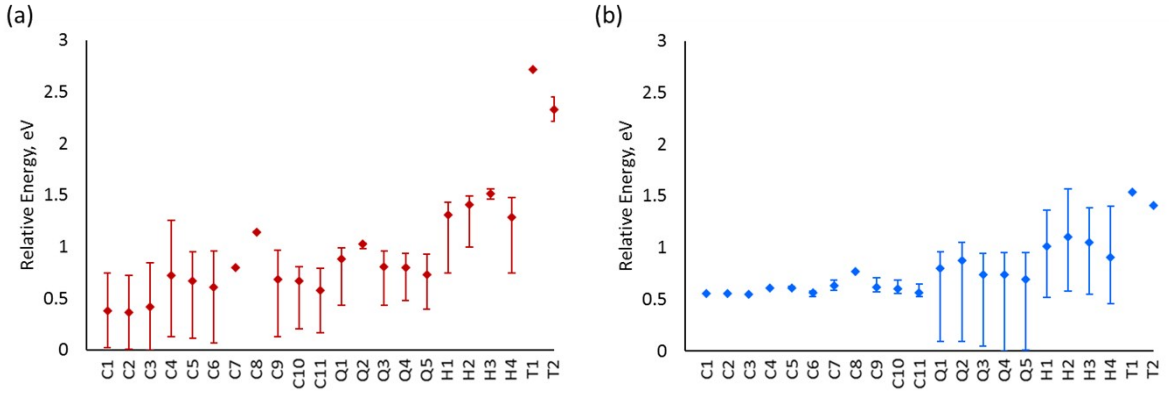

Figure S1: Average relative energies of anion orderings for (a) V_O-$BaNbO_2N$ and (b) V_N-$BaNbO_2N$. Bars above and below data points indicate minimum and maximum relative energy.

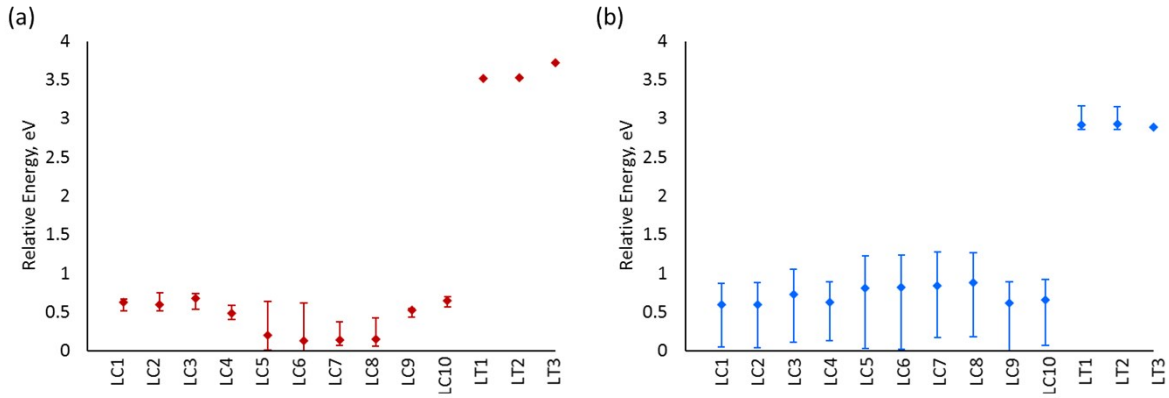

Figure S2: Average relative energies of anion orderings for (a) V_O-$LaNbON_2$ and (b) V_N-$LaNbON_2$. Bars above and below data points indicate minimum and maximum relative energy.

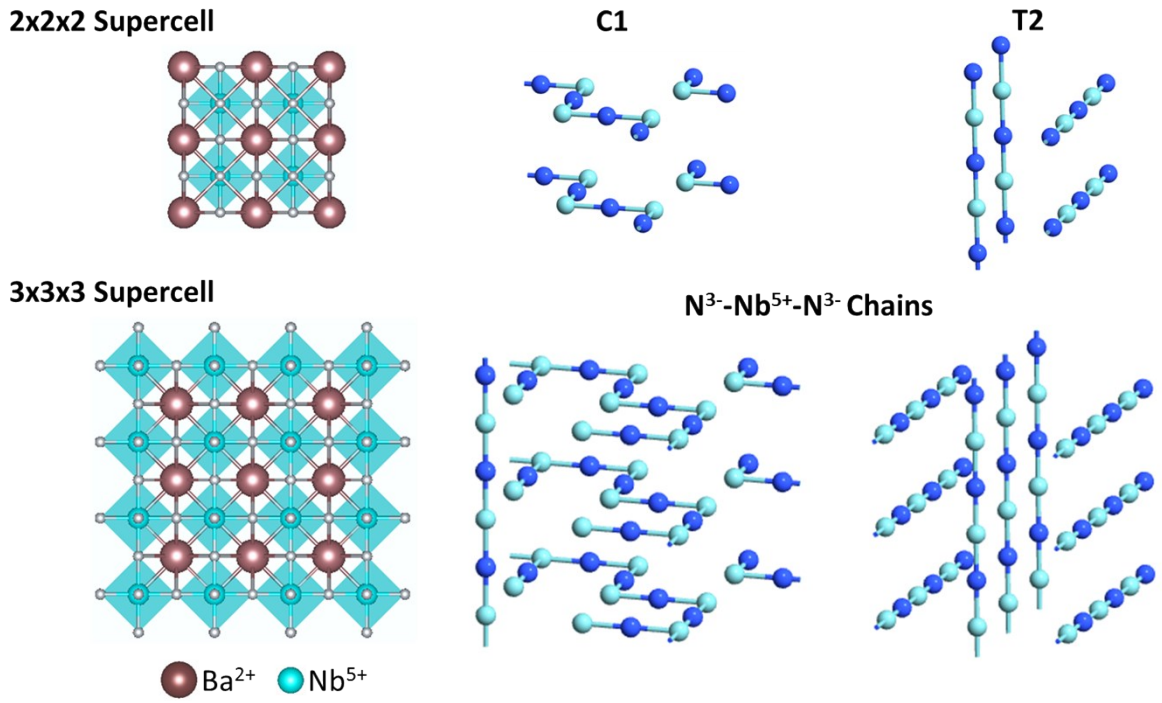

Figure S3: Translation of 2x2x2 $BaNbO_2N$ supercells to 3x3x3 supercells for Nudged Elastic Band (NEB) calculations. 3x3x3 cell is shifted in periodicity to maintain centroid from 2x2x2.

Table S1: Comparison of climbing image NEB barrier heights for 2x2x2 and 3x3x3 BaNbO2N supercells

Anion Ordering	**3x3x3 Cell**	**2x2x2 Cell**		**Path Type**
C1	$E_{barrier}$ (eV)	$E_{barrier}$ (eV)	Delta (3x3x3-2x2x2)	
N5 to N7	6.70	5.33	1.38	long
N7 to N12	1.53	1.70	-0.16	short
O1 to O2	1.28	1.28	0.00	short
O1 to O4	5.33	3.76	1.57	long
T2	$E_{barrier}$ (eV)	$E_{barrier}$ (eV)	Delta (3x3x3-2x2x2)	
N1 to N4	4.83	5.27	-0.44	long
O5 to O2	1.13	1.08	0.05	short
O5 to O7	4.69	2.82	1.87	long