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Published version

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Supporting information

Novel BaTiO$_3$-based, Ag/Pd compatible lead-free relaxors
with superior energy storage performance

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Figure S-1. Full-pattern refinement of $x\text{B}_{2/3}\text{MN-BT}$ ceramics
Figure S-2. P-E loop for BT ceramics at 60 kV cm$^{-1}$
Figure S-3. (a-f) The frequency-dependent dielectric properties for \( xB_{23}MN-BT \) \( (x=0.00\leq x \leq 0.10) \) ceramics.
Figure S-4. (a-f) The SEM image of thermal-etched surfaces for $xB_{2/3}M_N$-BT ($x=0.00 \leq x \leq 0.10$) ceramics.
Figure S-5. (a-d) Unipolar P-E loops under $E_{\text{max}}$ and (e-h) calculated energy storage properties ($W_{\text{rec}}$ and $\eta$) at different electric field for $x$B$_{23}$MN-BT ceramics.
Figure S-6. (a) Changes of $E_{\text{max}}$ and $\Delta P$ for $xB_{23}M$N-BT ceramics. (b) Change of $W_{\text{rec}}$ and $\eta$ as function of $x$ concentration.
Table S-1. Refined crystallography details for BT-xB$_{2/3}$MN ceramics.

| Composition / x | 0.00  | 0.02  | 0.04  | 0.06  |
|-----------------|-------|-------|-------|-------|
| GOF             | 1.31  | 2.19  | 1.34  | 1.55  | 1.86  |
| $R_{exp}$       | 9.03  | 16.25 | 6.75  | 7.79  | 8.02  |
| $R_{wp}$        | 11.84 | 39.59 | 9.08  | 12.05 | 14.99 |
| Space group     | $P4mm$| $Pm3m$| $P4mm$| $Pm3m$| $Pm3m$|
| Cell mass       | 233.19| 234.642| 233.57| 234.64| 235.73|
| Cell volume     | 64.40(4)| 64.49(4)| 64.52(7)| 64.69(4)| 64.93(4)|
| Crystal density | 6.013(4)| 6.023(4)| 6.018(8)| 6.023(4)| 6.029(9)|
| Lattice parameter a / Å | 3.9946(12)| 4.0144(8)| 3.9901(13)| 4.0144(8)| 4.0192(8)|
| Lattice parameter c / Å | 4.0358(12)| N/A | 4.0211(8)| N/A | N/A |
| c/a ratio       | 1.0103| N/A | 1.0083| N/A | N/A |

Refined atoms position details

| site | NP | x    | y    | z    | Atom   | Occ | Beq |
|------|----|------|------|------|--------|-----|-----|
| 0.00 | Ba | 1    | 0.000| 0.000| 0.000  | Ba+2| 1.00| 0.012|
|      | Ti | 1    | 0.500| 0.500| 0.5370 | Ti+4| 1.00| 0.019|
|      | O1 | 1    | 0.5000| 0.5000| -0.3700| O-2 | 1.00| 0.062|
|      | O2 | 2    | 0.5000| 0.0000| 0.5180 | O-2 | 1.00| 0.042|
| 0.02 | Ba | 1    | 0.000| 0.000| 0.000  | Ba+2| 0.980| 0.025|
|      | Ti | 1    | 0.5000| 0.5000| 0.5370 | Ti+4| 0.980| 0.033|
|      | O1 | 1    | 0.5000| 0.5000| -0.3700| O-2 | 1.00| 0.051|
|      | O2 | 2    | 0.5000| 0.0000| 0.5180 | O-2 | 1.00| 0.033|
| 0.04 | Ba | 1    | 0.000| 0.000| 0.000  | Ba+2| 0.960| 0.015|
|      | Ti | 1    | 0.5000| 0.5000| 0.5000 | Ti+4| 0.960| 0.015|
|      | O1 | 3    | 0.000| 0.5000| 0.5000 | O-2 | 1.00| 0.004|
| 0.06 | Ba | 1    | 0.000| 0.000| 0.000  | Ba+2| 0.940| 0.022|
|      | Ti | 1    | 0.5000| 0.5000| 0.5000 | Ti+4| 0.940| 0.025|
|      | O1 | 3    | 0.000| 0.5000| 0.5000 | O-2 | 1.00| 0.012|
Table S-2. Average grain size for xB_{2/3}MN-BT ceramics

| Composition | Average grain size / μm |
|-------------|-------------------------|
| x=0.00      | 25.2 ± 0.6              |
| x=0.02      | 16.6 ± 0.5              |
| x=0.04      | 7.2 ± 0.6               |
| x=0.06      | 2.8 ± 0.3               |
| x=0.08      | 2.4 ± 0.5               |
| x=0.10      | 2.3 ± 0.4               |