

Electronic Supplementary Information (ESI)

Cross-Substitution Effect of Tantalum on Visible-Light-Driven Water Oxidation Activity of BaNbO₂N Crystals Grown Directly by an NH₃-Assisted Flux Method

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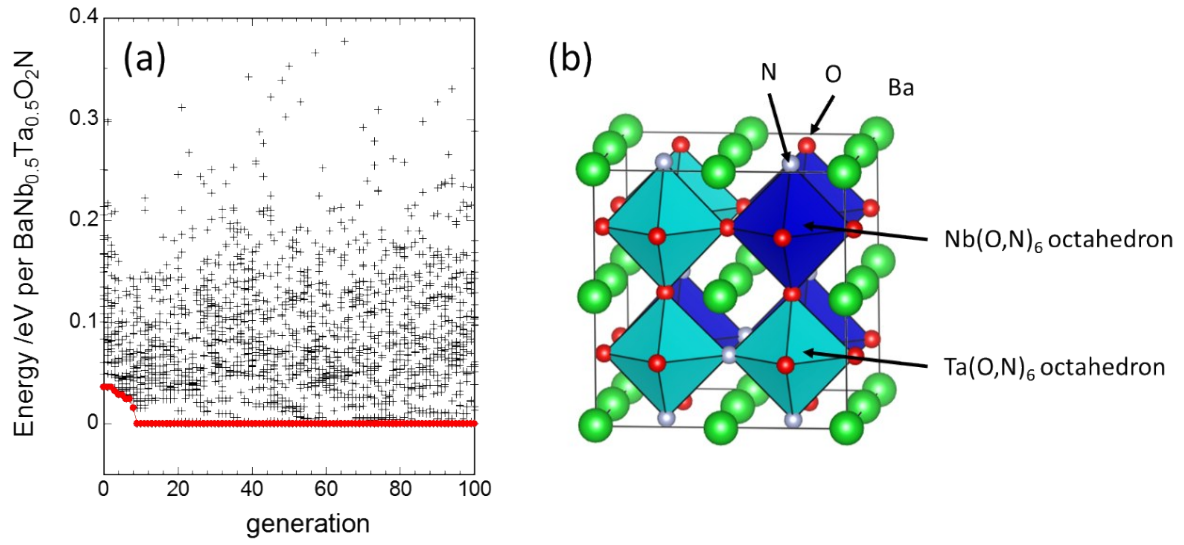


Figure S1. (a) Variation of total electron energies for genetic algorithm (GA)-driven structures as a function of generation (as an example of BaNb_{0.5}Ta_{0.5}O₂N). The red symbol indicates the lowest energy of GA-generated structures among present and previous generations. (b) Optimized Nb/Ta and O/N arrangement for BaNb_{0.5}Ta_{0.5}O₂N. The green, red and gray colored spheres correspond to Ba, O and N ions, respectively. The darker and lighter blue octahedra correspond to Nb(O,N)₆ and Ta(O,N)₆, respectively.

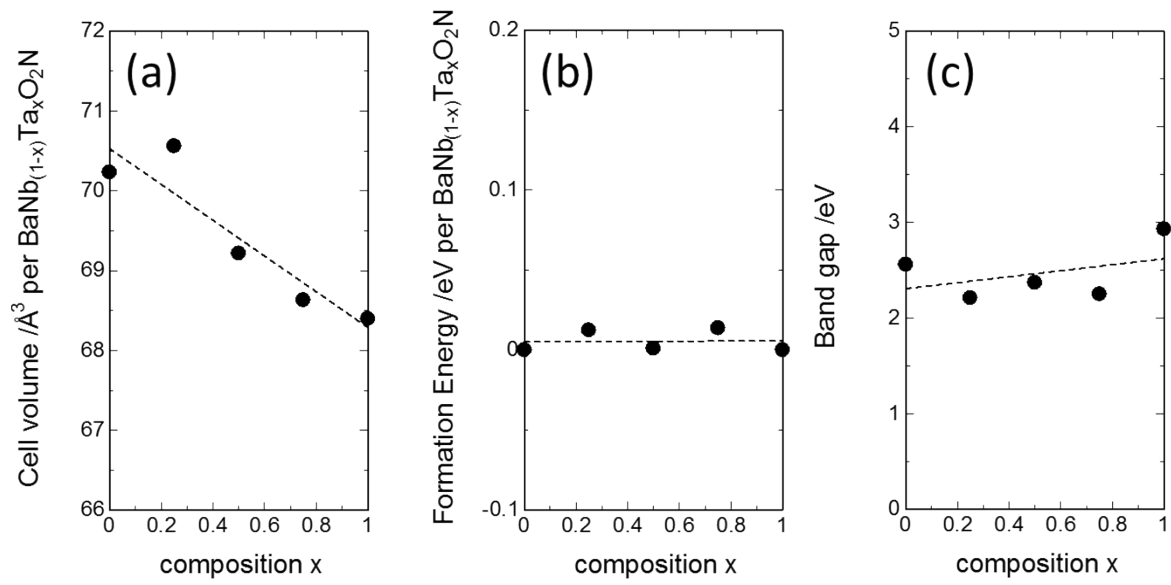


Figure S2. (a) Cell volume, (b) formation energy, and (c) band gap for $\text{BaNb}_{1-x}\text{Ta}_x\text{O}_2\text{N}$ as a function of x calculated by HSE06 functional.