

Perovskite BaTaO₂N: From Materials Synthesis to Solar Water Splitting

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Although hydrogen is a zero-emission energy carrier, its current global production still heavily relies on fossil fuels. Current momentum on renewable energy and environmental remediation is unprecedented because of fast climate change. We all know the world is hurrying to achieve the United Nations Sustainable Development Goals (SDGs) by 2030. One of the important SDGs is Goal 7: Affordable and Clean Energy. As a replica of natural photosynthesis, a semiconductor-based artificial photosynthetic system is regarded as one of the most economically viable, highly efficient, and environmentally benign chemical processes to generate green hydrogen energy from solar water splitting. However, to harness solar energy efficiently, it is necessary to enhance the visible-light-driven photocatalytic performance of the existing materials and to discover novel visible-light-active materials. Mixed-anion compounds offer new opportunities in this regard [1]. As a 600 nm-class photocatalyst, BaTaO₂N has received particular attention due to its small bandgap ($E_g = 1.8$ eV), suitable band edge positions for visible-light-induced water splitting, chemical stability, and nontoxicity [2,3]. BaTaO₂N is routinely synthesized by a two-step method: (i) the synthesis of a corresponding oxide precursor and (ii) its high-temperature nitridation under an NH₃ atmosphere for a prolonged period. However, this two-step method leads to the formation of various defects that negatively affect the water-splitting performance. Therefore, we have applied an NH₃-assisted direct flux growth approach to reduce the defect density of BaTaO₂N, engineered the bandgap by cation doping, and explored the effects of the altered morphology, size, and porosity on the visible-light-induced water oxidation activity and photoelectrochemical performance of BaTaO₂N. The findings revealed that the photocatalytic activity and photoelectrochemical performance of BaTaO₂N were significantly influenced by particle morphology, size, porosity, dopant type, and doping amount. Particularly, the BaTaO₂N crystal structures obtained by nitridation of the oxide precursor without KCl flux exhibited a higher surface area and high anodic photocurrents compared to the BaTaO₂N crystal structures obtained by nitridation of the oxide precursor with KCl flux due to the high number of dangling bonds acting as nucleation centers for the highly dispersed CoO_x cocatalyst nanoparticles.

References

- [1] H. Kageyama, K. Hayashi, K. Maeda, J. P. Attfield, Z. Hiroi, J. M. Rondinelli, K. R. Poeppelmeier, *Nat. Commun.* **2018**, *9*, 772.
- [2] R. Marchand, F. Pors, Y. Laurent, O. Regreny, J. Lostec, J. M. Haussonne, *J. Phys. Colloques* **1986**, *47*, C1-901.
- [3] M. Higashi, R. Abe, K. Teramura, T. Takata, B. Ohtani, K. Domen, *Chem. Phys. Lett.* **2008**, *452*, 120.