

Supplementary Information

Structural dependence of photocatalytic properties over double perovskite compound A_2InTaO_6 (A = Sr or Ba) doped with nickel

Meilin Lv^a, Yawei Wang^a, Lingwei Lu^a, Ruinan Wang^a, Shuang Ni^b, Gang Liu^c
and Xiaoxiang Xu^{a,*}

^aShanghai Key Lab of Chemical Assessment and Sustainability, Department of Chemistry, Tongji University, 1239 Siping Road, Shanghai, 200092, China

Email: xxxu@tongji.edu.cn, telephone: +86-21-65986919

^bScience and Technology on Plasma Physics Laboratory, Laser Fusion Research Center, China Academy of Engineering Physics, Mianyang 621900, China

^cShenyang National laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Science, 72 Wenhua Road, Shenyang 110016, China

Table of content

Fig. S1 Observed and calculated X-ray powder diffraction patterns of (a) $Ca_2In_{0.9}Ni_{0.1}TaO_6$, the refinement converged with good R -factors ($R_p = 5.41\%$, $R_{wp} = 7.67\%$, $\chi^2 = 2.943$). The refined crystal structure is shown in the inserted image.

Fig. S2 (a) UV-visible light absorption spectra (converted from diffuse reflectance spectra) of freshly prepared samples and (b) Kubelka-Munk transformation of diffuse reflectance data.

Fig. S3 (a) Temporal photocatalytic hydrogen production of all samples in aqueous sodium sulfite (0.05 M) under full range irradiation ($\lambda \geq 250$ nm), (b) average photocatalytic hydrogen production rate under full range irradiation ($\lambda \geq 250$ nm) and visible light irradiation ($\lambda \geq 400$ nm).

Table S1 Energy dispersive X-ray spectroscopy (EDS) analysis of as-prepared samples

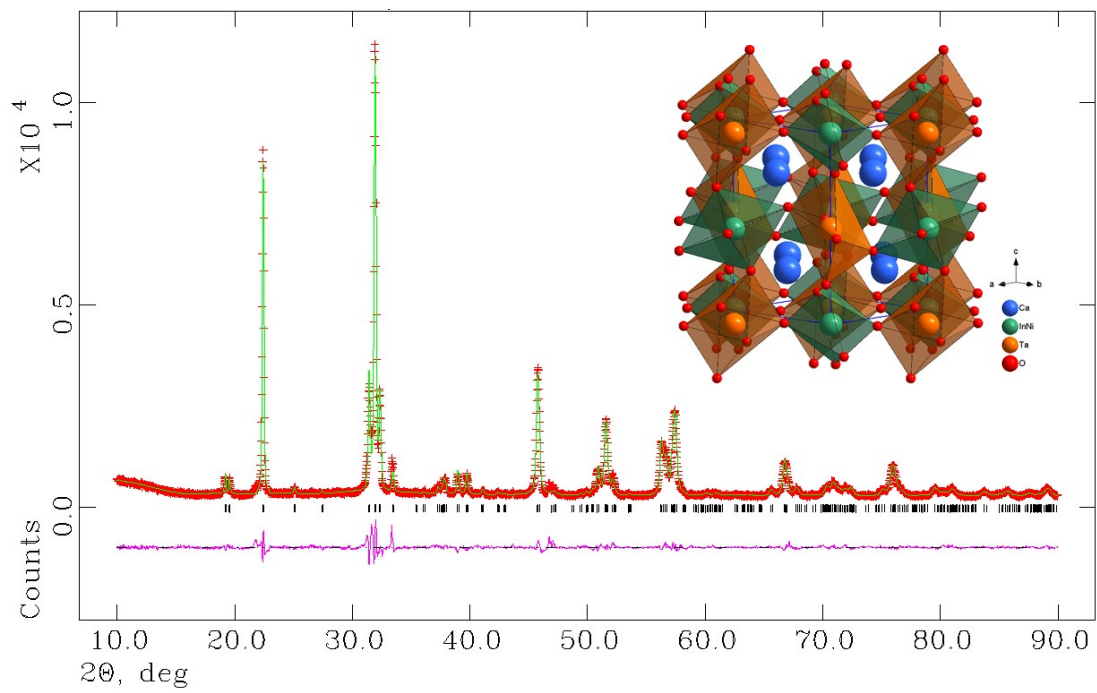


Fig. S1 Observed and calculated X-ray powder diffraction patterns of (a) $\text{Ca}_2\text{In}_{0.9}\text{Ni}_{0.1}\text{TaO}_6$, the refinement converged with good R -factors ($R_p = 5.41\%$, $R_{wp} = 7.67\%$, $\chi^2 = 2.943$). The refined crystal structure is shown in the inserted image.

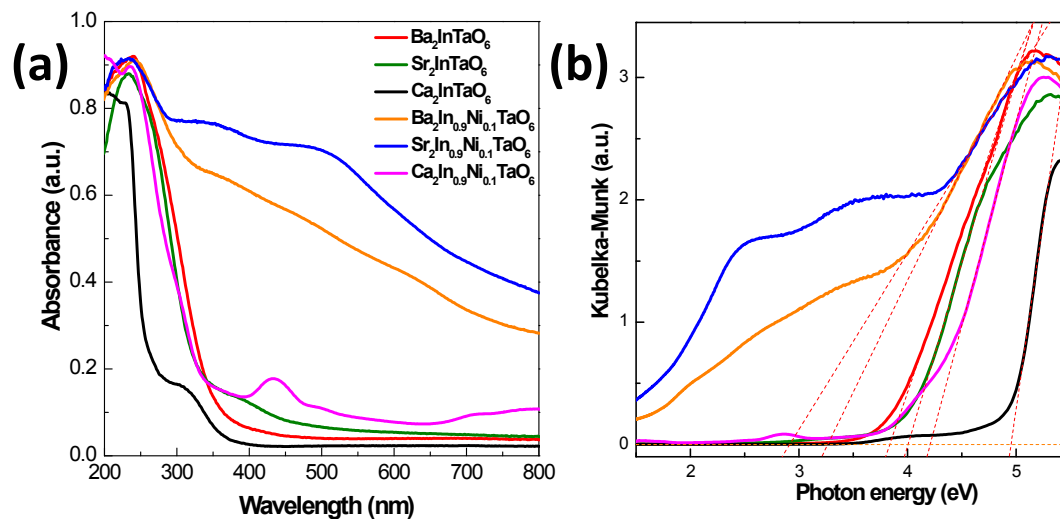


Fig. S2 (a) UV-visible light absorption spectra (converted from diffuse reflectance spectra) of freshly prepared samples and (b) Kubelka-Munk transformation of diffuse reflectance data.

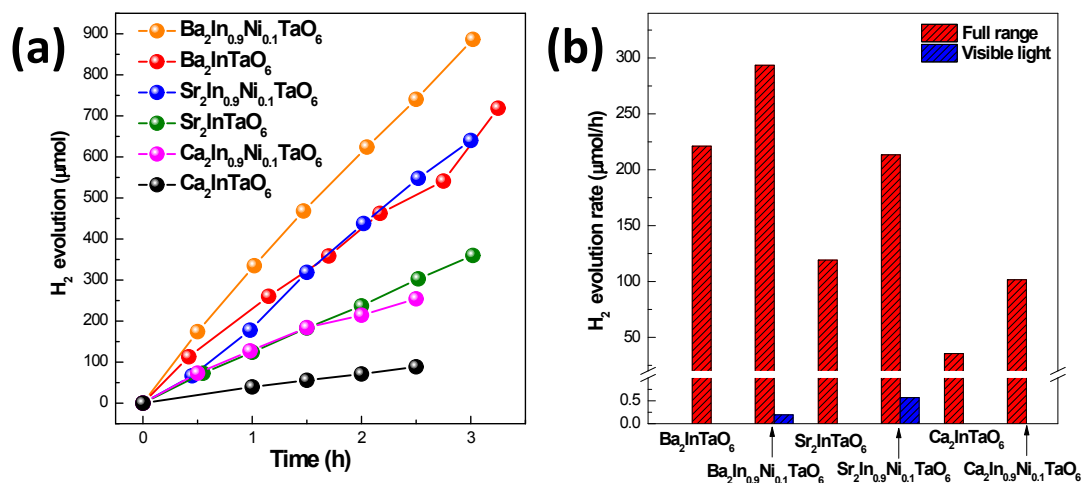


Fig. S3 (a) Temporal photocatalytic hydrogen production of all samples in aqueous sodium sulfite (0.05 M) under full range irradiation ($\lambda \geq 250$ nm), (b) average photocatalytic hydrogen production rate under full range irradiation ($\lambda \geq 250$ nm) and visible light irradiation ($\lambda \geq 400$ nm).

Table S1 Energy dispersive X-ray spectroscopy (EDS) analysis of as-prepared samples

| Samples | EDS analysis of as-prepared samples (mol%) | | | | |
|---|--|------|------|------|-------|
| | A | In | Ni | Ta | O |
| $\text{Ca}_2\text{InTaO}_6$ | 14.86 | 7.38 | - | 8.55 | 69.21 |
| $\text{Ca}_2\text{In}_{0.9}\text{Ni}_{0.1}\text{TaO}_6$ | 17.64 | 6.97 | 1.05 | 8.53 | 65.80 |
| $\text{Sr}_2\text{InTaO}_6$ | 16.80 | 8.03 | - | 7.80 | 67.37 |
| $\text{Sr}_2\text{In}_{0.9}\text{Ni}_{0.1}\text{TaO}_6$ | 17.87 | 7.69 | 0.72 | 8.20 | 65.52 |
| $\text{Ba}_2\text{InTaO}_6$ | 19.44 | 9.10 | - | 8.33 | 63.13 |
| $\text{Ba}_2\text{In}_{0.9}\text{Ni}_{0.1}\text{TaO}_6$ | 20.07 | 7.91 | 1.57 | 8.42 | 62.05 |