Supporting Information

Fabrication of Single-Crystalline BaTaO₂N from Chloride Fluxes for Photocatalytic H₂ Evolution under Visible Light

Ying Luo,^{†,}[♥] Zheng Wang,^{‡,}[♥] Sayaka Suzuki,[§] Kunio Yubuta,^{II} Nobuko Kariya,[⊥] Takashi Hisatomi,[‡] Kazunari Domen,^{*,‡,#} Katsuya Teshima^{*,‡,§}

[†]Department of Science and Technology, Graduate School of Medicine, Science and Technology, Shinshu University, 4-17-1 Wakasato, Nagano 380-8553, Japan

[‡]Research Initiative for Supra-Materials, Shinshu University, 4-17-1 Wakasato, Nagano 380-8553, Japan

[§]Department of Materials Chemistry, Faculty of Engineering, Shinshu University, 4-17-1 Wakasato,

Nagano 380-8553, Japan

^{II} Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

¹Science & Innovation Center, Mitsubishi Chemical Corporation, 1000 Kamoshida-cho, Aoba-ku, Yokohama, Kanagawa 227-8502, Japan

[#]Office of University Professor, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656,

Japan

^vThese authors contributed equally

*Corresponding Authors: K.T., K.D

E-mail address: teshima@shinshu-u.ac.jp, domen@chemsys.t.u-tokyo.ac.jp



Figure S1. Synthetic route to the BaTaO₂N crystals.



Figure S2. (a) XRD pattern and (b) SEM image of BTON (BaCl₂) prepared using a solute concentration of 10 mol%.



Figure S3. Ta 4f XPS spectra of BTON (RbCl), BTON (CsCl), and BTON (BaCl₂).



Figure S4. XRD patterns of BTON (RbCl) prepared using holding temperatures of 900, 950, and 1000 °C.



Figure S5. SEM images of BTON (RbCl) prepared using holding temperatures of (a) 900,

(b) 950, and (c) 1000 °C.



Figure S6. UV-vis DRS of BTON (RbCl) prepared using holding temperatures of 900, 950, and 1000 °C.



Figure S7. Ta 4f XPS spectra of BTON (RbCl) prepared using holding temperatures of 900, 950, and 1000 °C.



Figure S8. XRD patterns of BTON (RbCl) prepared using holding times of 6, 8, and 10

h.



Figure S9. SEM images of BTON (RbCl) prepared using holding times of (a) 6, (b) 8,

and (c) 10 h.