### Supporting Information for

# Quasi-linear Dependence of Cation Filling on the Photocatalysis of A<sub>x</sub>BO<sub>3</sub>-Based Tunnel Compounds

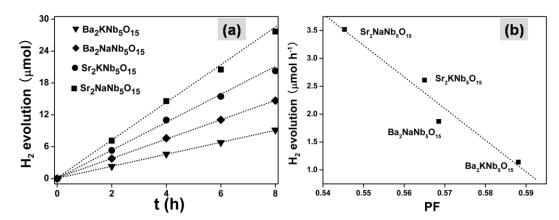
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#### 1. Photocatalytic hydrogen evolution measurements

Figure S1 (a) Photocatalytic H<sub>2</sub> evolution from CH<sub>3</sub>OH–H<sub>2</sub>O solution over  $(A1)_2(A2)$ Nb<sub>5</sub>O<sub>15</sub> (A1 = Sr, Ba; A2 = Na, K) under UV light irradiation (Cat: 0.6 g, CH<sub>3</sub>OH: 50 mL, H<sub>2</sub>O: 250 mL). (b) The obtained nearly-linear correlation \*

\* Photocatalytic hydrogen evolution from aqueous solution containing methanol used as a sacrificial reagent for  $h^+$  capture. A nearly-linear correlation is also obtained.

### 2. Photocatalytic degradation of other substrates

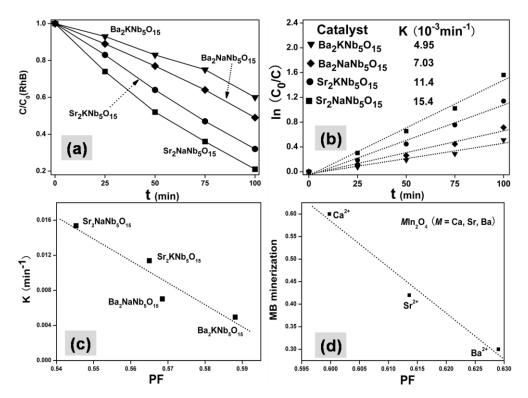


Figure S2 (a) Photodegradation of RhB over  $(A1)_2(A2)Nb_5O_{15}$  (A1 = Sr, Ba; A2 = Na, K) under UV light irradiation. (b) Reaction kinetics of RhB decomposition. The obtained nearly-linear correlation from (c) Photodegradation of RhB over  $(A1)_2(A2)Nb_5O_{15}$  (A1 = Sr, Ba; A2 = Na, K) in this work, and (d) MB mineralization from over  $MIn_2O_4$  (M = Ca, Sr, Ba) in ref. 20 \*

\* The concentrations of RhB during the catalytic reactions were determined by monitoring the changes of the main absorbance maximized at 554 nm. The volume of the initial 10.0 mg/L RhB aqueous solution is 300 mL (Fig. S2 a-c). Actually, in the ref. 20 presented in this manuscript, the same conclusion was also obtained in the case of another organic dye, methyl blue (MB) (As shown in Fig. S2 d). The catalytic efficiency of each system also exhibits a quasi-linear dependence on the cation filling of crystal structure (or PF).

## 3. The effect of catalyst concentration on MO photodegradation efficiency

In order to determine the optimal catalyst concentration, a series of experiments with varied catalyst concentration  $(0.25\sim4 \text{ g/L})$  have been conducted (Take

Sr<sub>2</sub>KNb<sub>5</sub>O<sub>15</sub> as example). The effect of catalyst concentration on the photodegradation

efficiency was shown in Fig. S3.

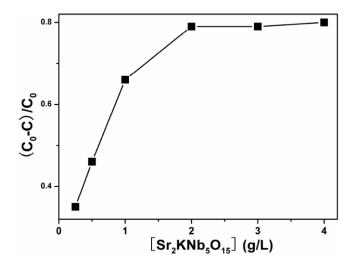


Fig. S3 Dependences of MO photodegradation efficiency on catalyst concentration, where the efficiency of  $(C_0-C)/C_0$  was recorded after UV-light irradiation for 80 min.\*

\* The photodegradation rate of methyl orange (MO) increases with increasing catalyst concentration and reaches a maximum at 2 g/L, after which the rate becomes constant. This observation can be explained in terms of availability of active sites on the catalyst surface and the penetration of UV light into the suspension. The total active surface area increases with increasing catalyst dosage. Meanwhile, due to an increase in the turbidity of the suspension, there is a decrease in UV light penetration as a result of increased scattering effect and hence the photoactivated volume of suspension decreases. So the 2 g/L used here serves as an optimization in the present manuscript.

#### 4. Methyl orange adsorption on the as-investigated compounds

In our control experiments, the surface adsorption percentage after 4 h is 5.2%, 4.4%, 4.7% and 4.5% for  $Ba_2KNb_5O_{15}$  (BKN),  $Ba_2NaNb_5O_{15}$  (BNN),  $Sr_2KNb_5O_{15}$  (SKN) and  $Sr_2NaNb_5O_{15}$  (SNN) respectively, indicating that the adsorption difference should not be responsible for the photocatalysis discrepancy observed during the tests.

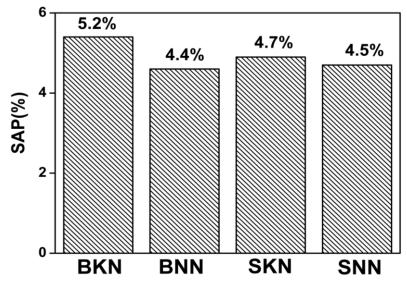


Fig. S4 SAP =  $(C_0 - C)/C_0 * 100\%$ , where  $C_0$  is the initial MO concentration and C is the concentration after 4 h adsorption.