

## Electronic Supplementary Information (ESI)

### Photocatalytic NO removal over calcium-bridged siloxenes under ultraviolet and visible light irradiation

Haruo Imagawa,<sup>a\*</sup> Xiaoyong Wu,<sup>b</sup> Hiroshi Itahara,<sup>a</sup> Shu Yin,<sup>b</sup> Kazunobu Kojima,<sup>b</sup> Shigefusa F.

Chichibu<sup>b</sup> and Tsugio Sato<sup>b</sup>

<sup>a</sup>Toyota Central R&D Labs., Inc. 41-1 Yokomichi, Nagakute, Aichi, 480-1192 Japan.

<sup>b</sup>Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan.

E-mail: [e1152@mosk.tytlabs.co.jp](mailto:e1152@mosk.tytlabs.co.jp)

#### 1. X-ray diffraction (XRD) data of Ca-siloxenes (Fig. S1)

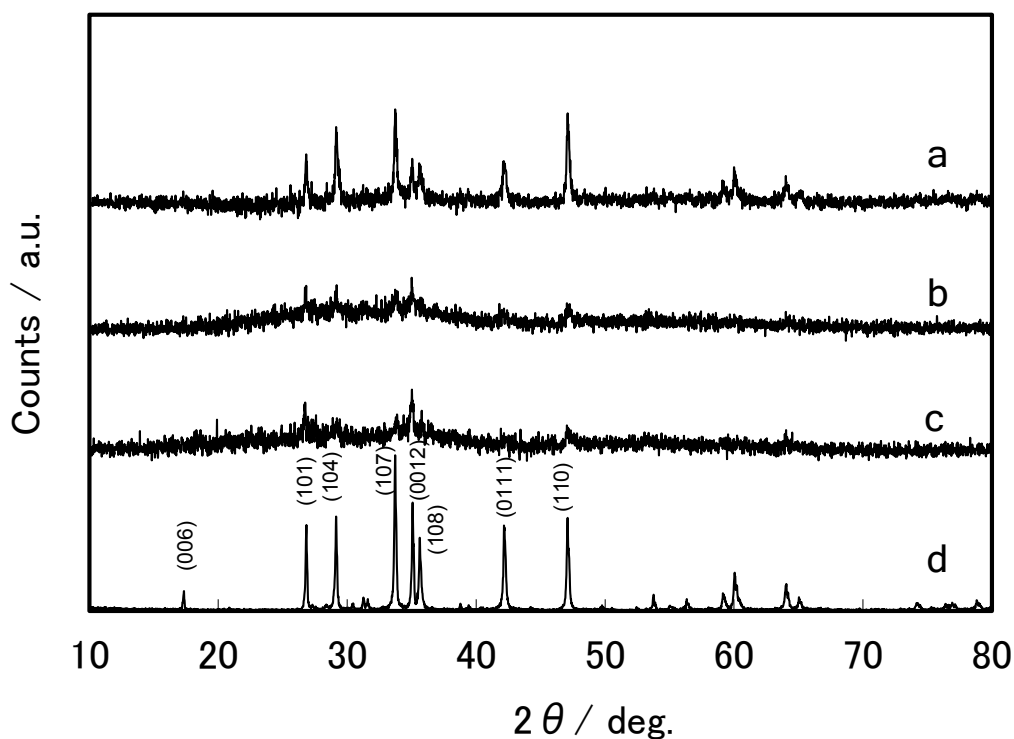


Fig. S1. XRD patterns of (a) CS2.5, (b) CS1.25, (c) CS0.25, and (d) CaSi<sub>2</sub>.

## 2. Apparent quantum efficiency (Fig. S2)

The apparent quantum efficiency was calculated based on the following equation :

$$\Phi(\%) = 100 \times F_{\text{NO}}\alpha_{\lambda}/P_{\lambda}SA_{\lambda},$$

where  $F_{\text{NO}}$  ( $\mu\text{mol s}^{-1}$ ) is the NO amount rate in the feed gas,  $\alpha_{\lambda}$  is NO conversion of samples (%),  $P_{\lambda}$  ( $\mu\text{mol s}^{-1}$ ) is the light intensity on the surface of sample holder ( $\lambda > 290 \text{ nm}$ :  $1139.8 \text{ } (\mu\text{mol s}^{-1})$ ,  $> 400 \text{ nm}$ :  $846.7 \text{ } (\mu\text{mol s}^{-1})$ ),  $S$  is the surface area of sample holder ( $1.28 \times 10^{-3} \text{ m}^2$ ), and  $A_{\lambda}$  is the average light absorption ratio of samples at different light wavelength based on UV/visible absorption spectra.

Average light absorption ratio:  $\lambda > 290 \text{ nm}$  : CS0.25-93.1%、CS1.25-93.4%、CS2.5-86.6%、 $\lambda > 400 \text{ nm}$  : CS0.25-93.1%、CS1.25-92.8%、CS2.5-85.8%.

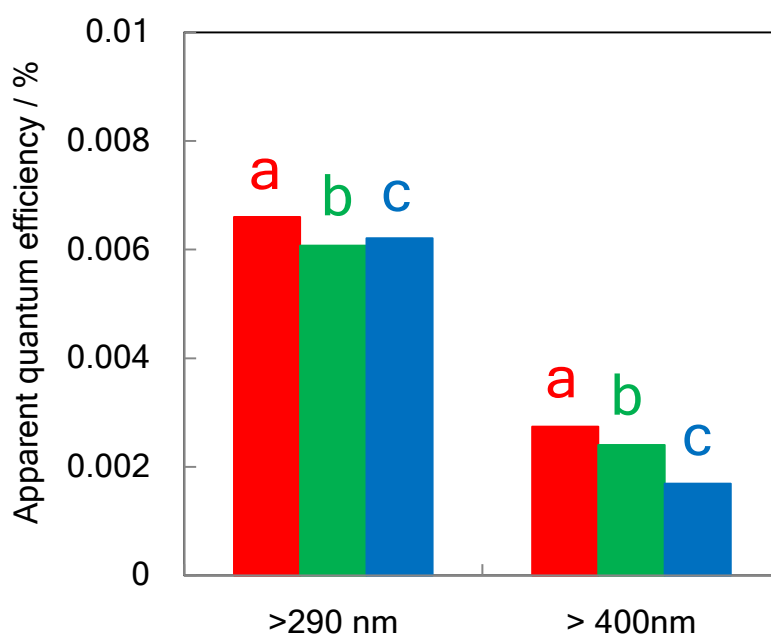


Fig. S2. Apparent quantum efficiency irradiated at  $\lambda > 290 \text{ nm}$   $> 400 \text{ nm}$  with 10 wt% acetylene black:(a) CS0.25, (b) CS1.25, and (c) CS2.5.