

Masashi Morita, Hikaru Inada and Kazuyuki Maeda

Department of Applied Chemistry, Graduate School of Engineering,  
Tokyo University of Agriculture and Technology, 2-24-16 Naka-  
cho, Koganei, Tokyo 184-8588, Japan.

E-mail: m-morita@go.tuat.ac.jp



### Stabilization of molecular $\text{TiO}_4$ species on the pore surface of mesoporous silica and its photocatalytic properties

Although molecular tetrahedral Ti-oxo species exhibit unique electronic and photochemical properties due to their discrete energy levels,<sup>1</sup> which are different from those of anatase and rutile, such Ti-oxo species are generally unstable and readily transformed to amorphous/crystalline  $\text{TiO}_2$  (bulk phases, nanoparticles, and clusters) via hydrolysis and condensation. Here, molecular Ti-oxo species were immobilized on the pore surface of mesoporous silica SBA-15 by grafting titanium(IV) oxyacetylacetonate using the surface silanol groups of SBA-15 as a scaffold, followed by chemical etching with dilute hydrochloric acid to form molecular  $\text{TiO}_4$  species.<sup>2</sup> These Ti species mainly exist as isolated tetrahedrally coordinated structures, as was confirmed by diffuse reflectance UV-vis and Raman spectroscopy. The SBA-15-immobilized molecular  $\text{TiO}_4$  exhibited higher photocatalytic activity than the reference photocatalysts (P25 and Ti-MCM-41) for both  $\text{H}_2$  production from methanol solution and  $\text{CO}_2$  reduction to  $\text{C}_2$  products such as ethanol and acetic acid.

#### References:

- [1] H. Yamashita, K. Mori, Y. Kuwahara, T. Kamegawa, M. Wen, P. Verma and M. Che, *Chem. Soc. Rev.*, **47**, 8072 (2018).
- [2] H. Inada, M. Morita and K. Maeda, *Dalton Trans.*, 53, 13756 (2024).