Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2021

ESI for

# Catalytic epoxidation of $\beta$ -ionone epoxidation with molecular oxygen on selenium-doped silica

Peizi Li<sup>a</sup>, Kuanhong Cao<sup>a</sup>, Xiaobi Jing<sup>a</sup>, Yonghong Liu<sup>a,\*</sup>, and Lei Yu<sup>a,\*</sup>

<sup>a</sup>School of Chemistry and Chemical Engineering, Yangzhou University, Yangzhou,

Jiangsu 225002, China

Fax: +86 514 87975244; Tel: +86 136 65295901; Emails: <u>yhliu@yzu.edu.cn</u> (Y. Liu); <u>yulei@yzu.edu.cn</u> (L. Yu)

# CONTENTS

FT-IR spectra of the materials	.S2
XRD patterns of the materials	.S3
XPS details	.S4
XPS spectrum of Se/SiO <sub>2</sub> -F on F	
EDX spectrum of Se/SiO <sub>2</sub> -F	.S5
<sup>1</sup> H NMR data and spectrum of $\beta$ -ionone epoxide	.S6

### FT-IR spectra of the materials



Fig. S1. FT-IR spectra of the materials.

## XRD patterns of the materials



Fig. S2. XRD pattern of Se/SiO<sub>2</sub>-KF.



Fig. S3. XRD pattern of Se/SiO<sub>2</sub>.



Fig. S4. XRD pattern of SiO<sub>2</sub>-KF.

#### **XPS** details

ESCALAB 250Xi of Thermo Fisher Scientific with mono AI K $\alpha$  (1486.6 eV) was employed. When the neutralization gun was turned on in the whole process, the test beam spot size was 500  $\mu$ m under standard mode (CAE). Full spectrum passing energy was 150 eV, with step size at 1.0 eV; Narrow spectrum passing energy was 30 eV, with step size at 0.05 eV. The sample was pre-vacuumized to  $2.0 \times 10^{-8}$  mbar in

the injection chamber and transferred to the analysis chamber of  $9.0 \times 10^{-10}$  mbar step

by step. In the actual test, the vacuum was  $3.0 \times 10^{-7}$  mbar because the neutralization

gun was turned on.

Chemical state	Binding energy Si 2p/eV
Organic Si	102 (References:1)
SiO <sub>2</sub>	103.5 (References:1)

Chemical state	Binding energy Se 3d/eV
Se	55.2 (Ref. 1)
Se <sup>4+</sup>	59.07 (Ref. 2)

References:

1. https://srdata.nist.gov/xps/selEnergyType.aspx

2. S. Zhu, J. Hu, S. Liu. Carbohyd. Polym. 246 (2020) 116545.

XPS spectrum of Se/SiO<sub>2</sub>-F on F



Fig. S5. XPS spectrum of Se/SiO<sub>2</sub>-F on F.

EDX spectrum of Se/SiO<sub>2</sub>-F



Fig. S6. EDX spectrum of Se/SiO<sub>2</sub>-F.

### <sup>1</sup>H NMR data and spectrum of $\beta$ -ionone epoxide

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.00 (d, *J* = 15.7 Hz, 1H), 6.27 (d, *J* = 15.6 Hz, 1H), 2.26 (s, 3H), 1.88 (dq, *J* = 9.9, 7.9 Hz, 1H), 1.74 (dt, *J* = 14.7, 5.3 Hz, 1H), 1.48 – 1.37 (m, 3H), 1.13 (s, 6H), 1.06 (ddd, *J* = 10.9, 5.3, 2.2 Hz, 1H), 0.92 (s, 3H). Known product [Catal. Sci. Technol. 8 (2018) 5017–5023].

