ESI for

Highly crystalline K-intercalated Se/C: An easily accessible mesoporous material catalyzing the epoxidation of *β*-ionone

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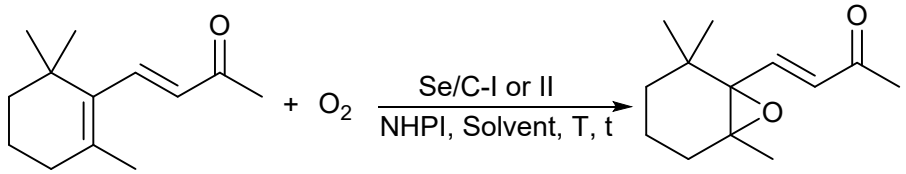
Table S1 Optimization of the reaction conditions of Se/C-catalyzed *β*-ionone epoxidation[a]

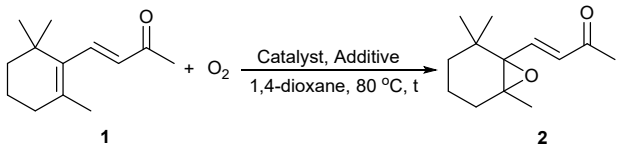


1 **2**

Entry	Cat.	Solvent	T (°C)	t (h)	Conversion (%)	Selectivity (%)	Yield (%)[c]	TON (mol/mol)
1	I	MeCN	80	24	78	45	35	6.31×10^3
2	II	MeCN	80	24	58	28	16	4.45×10^3
3	I	EtOH	80	24	81	32	26	4.69×10^3
4	I	EtOAc	80	24	63	27	17	3.07×10^3
5	I	DMC	80	24	60	33	20	3.61×10^3
6	I	THF	80	24	55	20	11	1.98×10^3
7	I	1,4-dioxane	80	24	94	65	61	1.10×10^4
8	I	1,4-dioxane	60	24	56	77	43	7.75×10^3
9	I	1,4-dioxane	100	24	99	20	20	3.61×10^3
10	I	1,4-dioxane	80	12	59	66	39	7.03×10^3
11	I	1,4-dioxane	80	36	99	21	21	3.79×10^3

[a] 1 mmol of **1**, 0.1 mmol of NHPI, 20 mg of catalyst, and 1 mL of solvent were employed. [b] Isolated yield of **2** based on **1**.

Table S2 Control experiments for mechanism study[a]



Entry	Catalyst; Additive[b]	t (h)	Conversion (%)	Selectivity (%)	Yield (%)[c]	TON (mol/mol)
1	Se/C-I (20 mg); none	24	64	63	40	7.21×10^3
2	Se/C-I (40 mg); none	24	66	49	32	5.77×10^3
3	Se/C-I (20 mg); NHPI (10%)	24	94	65	61[d]	1.10×10^4
4	None; NHPI (10%)	24	34	69	23	-
5	None; NHPI (20%)	24	39	67	26	-
6	KBr (5%), NHPI (10%)	24	22	78	17	-
7	MgO (5%), NHPI (10%)	24	26	81	21	-
8	Se/C-I (20 mg); NHPI (10%) and AIBN (100%)	6	55	71	39	7.03×10^3
9	Se/C-I (20 mg); NHPI (10%)	12	59	66	39[d]	7.03×10^3
10	Se/C-I (20 mg); NHPI (10%) and	24	23	69	16	2.89×10^3

	TEMPO (100%)					
11	Se/C-II (20 mg); NHPI (10%)	24	42	52	22	6.12×10^3
12	Se/C-II (40 mg); NHPI (10%)	24	56	45	25	3.48×10^3

[a] 1 mmol of **1**, 20 mg of Se/C-I (if used), and 1 mL of 1,4-dioxane were employed. [b] Weight amount of the catalyst or molar ratio of the additive vs. **1** was gave inside the parentheses; [c] Isolated yield of **2** based on **1**; [d] Data in entries 3 and 9 in this table were from the Table S1, entries 7 and 10 respectively.

Details of quantitative calculations

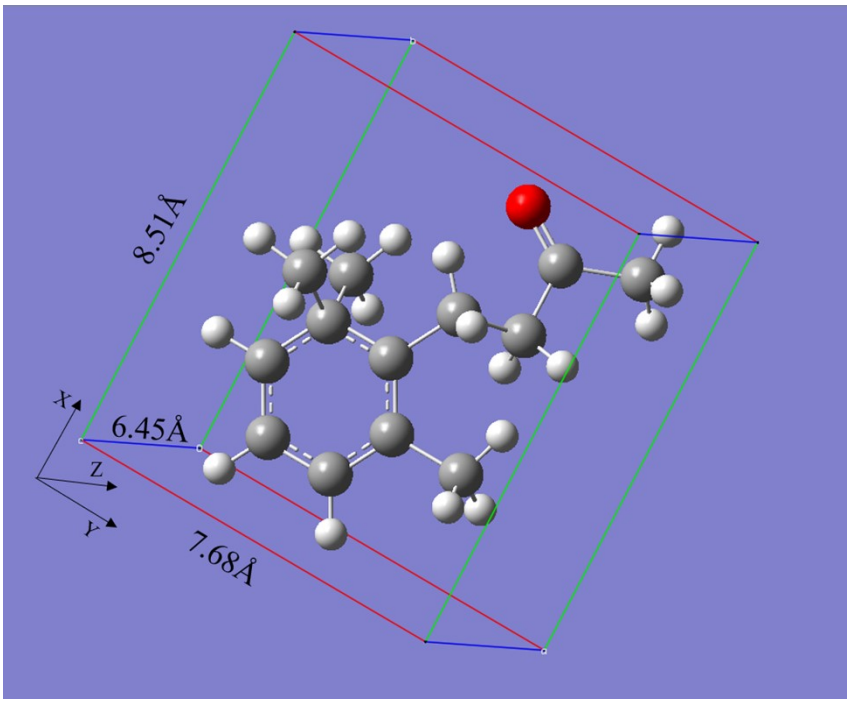


Fig. S1 Space structure of *β*-ionone.

The calculation process of maximum length of cuboid that can hold *β*-ionone molecule (The length, width and height values of the cuboid are all from GaussView 5 software using density functional theory (DFT) at B3PW91/6-311G level):

$$X_1 = 8.51 \text{ Å}$$

$$Y_1 = 7.68 \text{ Å}$$

$$Z_1 = 6.45 \text{ Å}$$

$$L_{1\,max} = \sqrt{(X_1^{\,2} + Y_1^{\,2} + Z_1^{\,2})} = 13.15 \text{ Å} = 1.32 \text{ nm} < 3.2 \text{ nm}$$

Thus, *β*-ionone molecule can enter the catalyst pores freely.

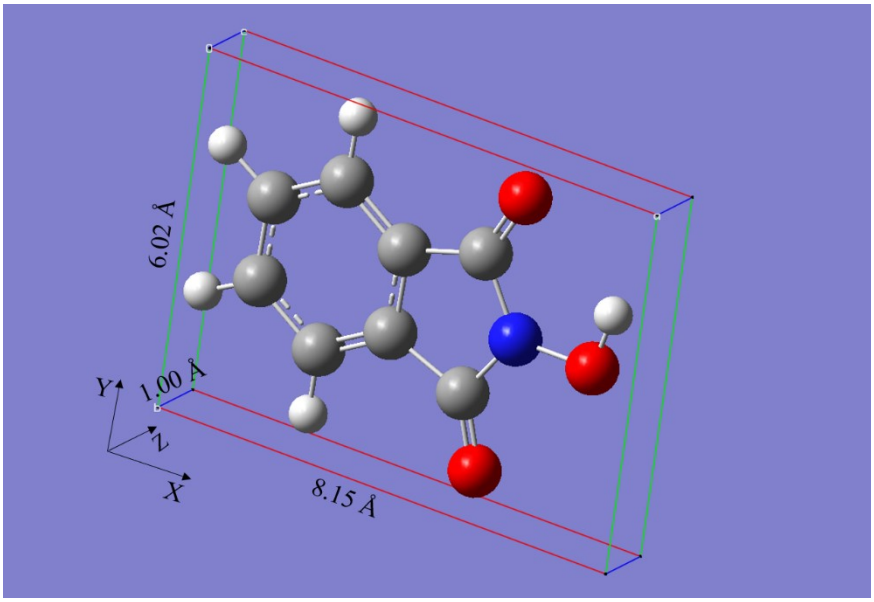


Fig. S2 Space structure of NHPI.

The calculation process of maximum length of cuboid that can hold NHPI molecule (The length, width and height values of the cuboid are all from GaussView 5 software using density functional theory (DFT) at B3PW91/6-31G level):

$$X_2 = 8.15 \text{ Å}$$

$$Y_2 = 6.02 \text{ Å}$$

$$Z_2 = 1.00 \text{ Å}$$

$$L_{2\,max} = \sqrt{(X_2^{\,2} + Y_2^{\,2} + Z_2^{\,2})} = 10.18 \text{ Å} = 1.02 \text{ nm} < 3.2 \text{ nm}$$

Thus, NHPI molecule can also enter the catalyst pores freely.

Enlarged figures

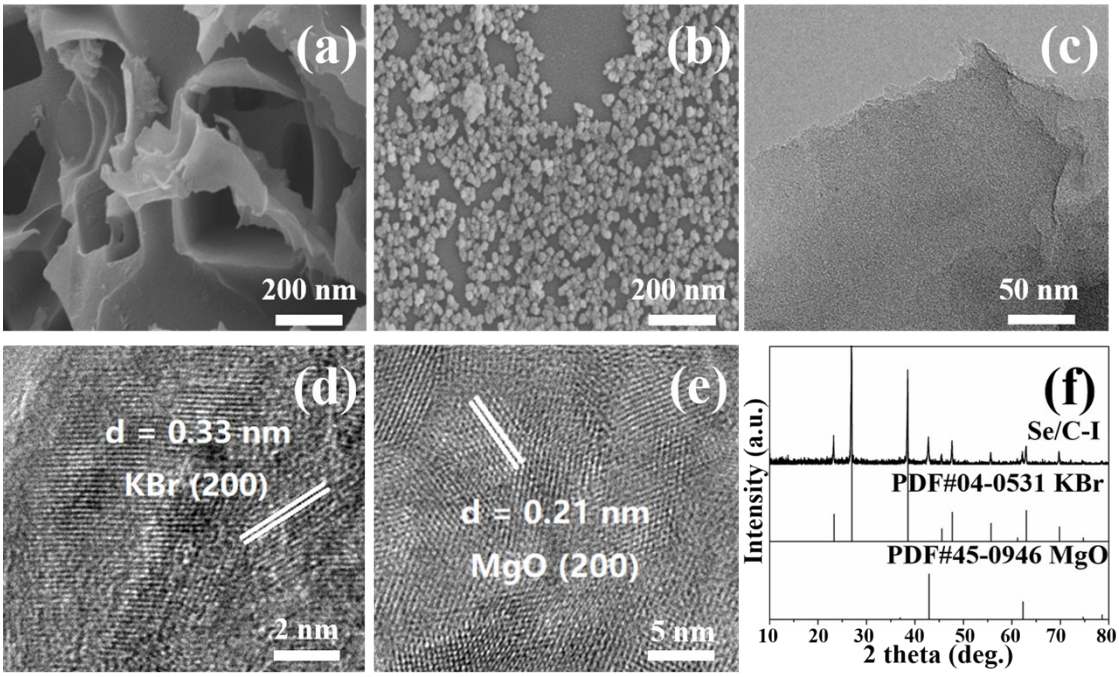


Fig. S3 (Fig. 1 in text) Characterization of the materials (*a*) SEM image of Se/C-I; (*b*) SEM image of Se/C-II; (*c*) TEM image of Se/C-I; (*d*,*e*) HRTEM images of Se/C-I; (*f*) XRD pattern of Se/C-I.

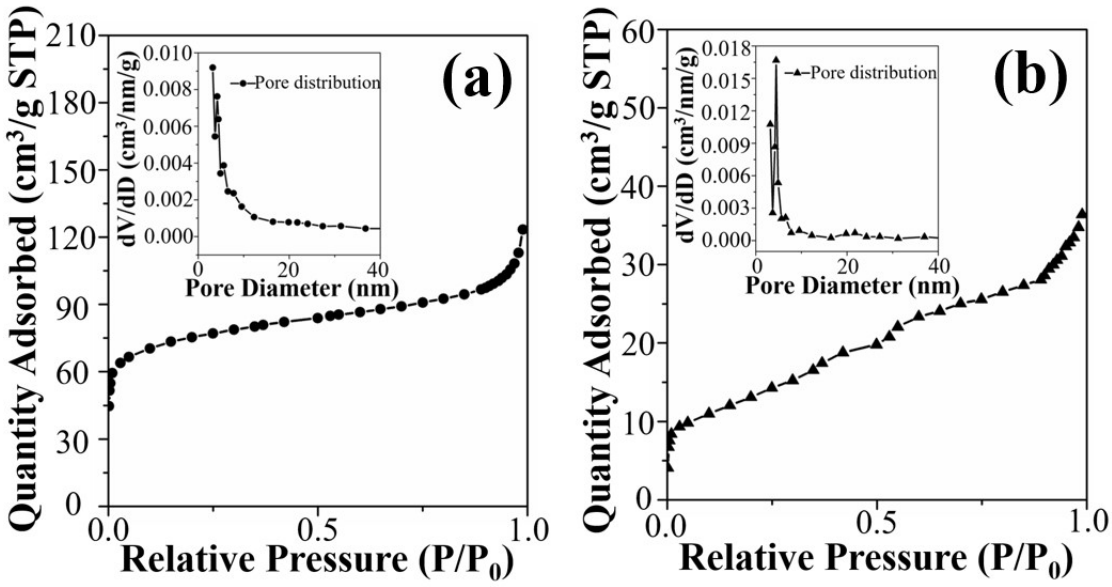
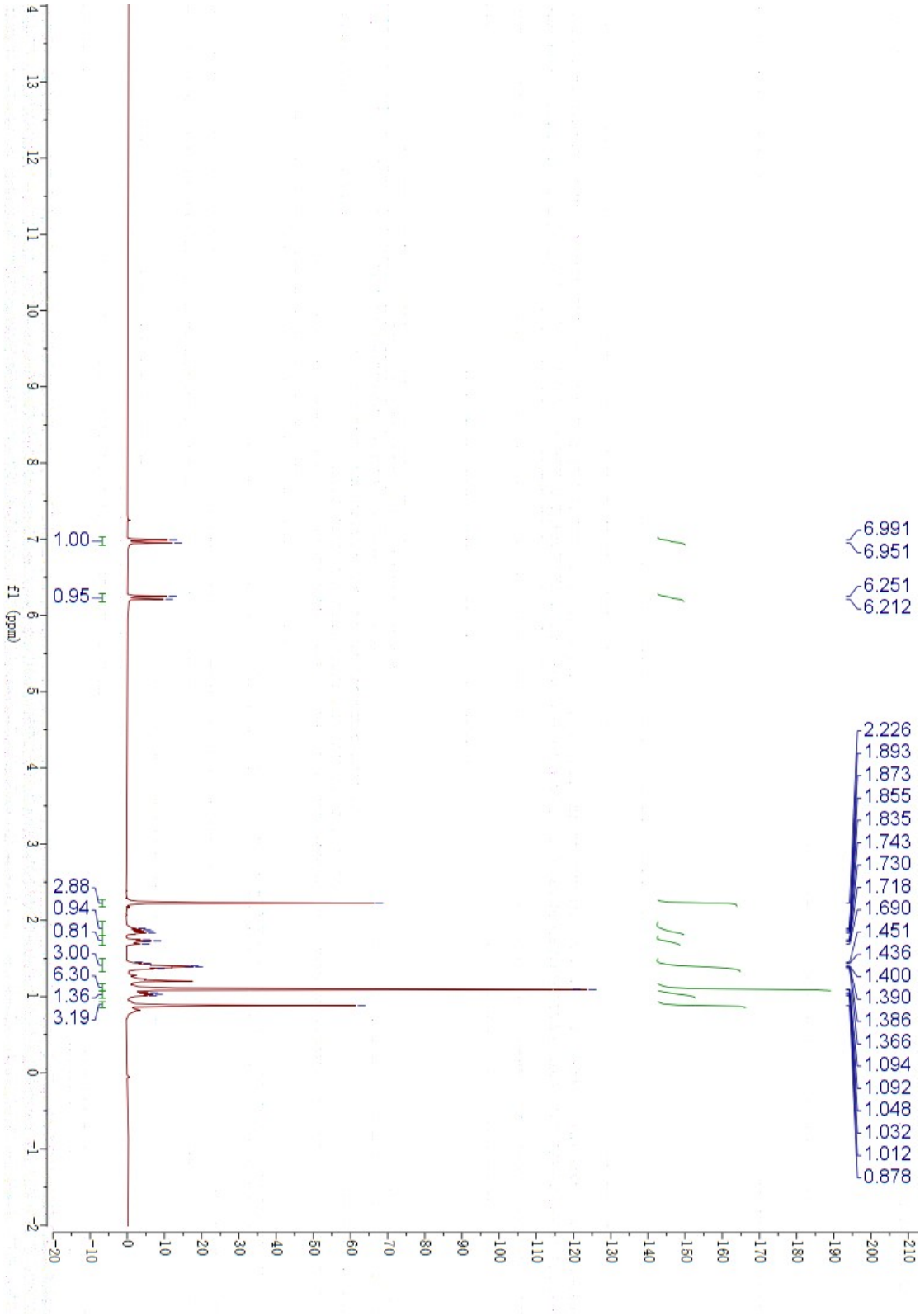


Fig. S4 (Fig. 4 in text) Nitrogen adsorption-desorption isotherms of Se/C-I and II.

NMR spectrum of the product 2

2, ^{1}H NMR, $CDCl_3$, 400 MHz



2, ^{13}C NMR, $CDCl_3$, 100 MHz