Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information

Development of a novel theory of pressure-induced nucleation in supercritical carbon dioxide

Qi-Bo Wang, Qin-Qin Xu*, Jian-Zhong Yin, Hong-Yue Zhu, Bao-Lin Liu, Ming-Zhe Yang

State Key Laboratory of Fine Chemicals, School of Chemical Engineering, Dalian University of Technology, Dalian 116024, China

Table S1 Data of $MoO_2(acac)_2$ mole fraction y_1 in $scCO_2$

Temperature (℃)	Pressure (MPa)	Density of $scCO_2$ ($kg \cdot m^{-3}$)	$y_1 \times 10^4$
40	7.4	233.38	1.818
	10.0	631.74	0.809
	12.0	719.38	1.033
	14.4	764.47	1.236
	16.0	795.91	1.315
	18.0	820.39	1.485
	20.0	840.61	1.604
50	7.4	188.78	1.420
	10.6	460.74	1.350
	12.0	587.07	2.026
	14.0	673.7	2.535
	16.0	723.27	2.894
	18.0	758.11	3.754
	20.0	785.16	4.172
60	7.4	168.75	1.316
	10.0	290.81	1.821
	12.0	436.26	2.006
	14.0	563.09	2.830
	16.0	638.84	3.761
	18.0	688.34	4.128
	20.0	724.63	4.829

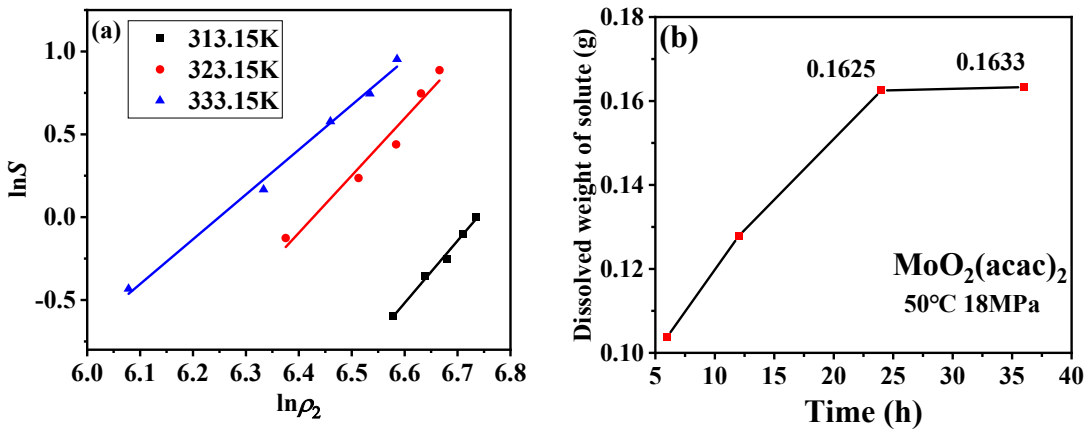

Fig. S1 (a) Linear relationships between the logarithms solubility and the logarithms density of $scCO_2$ at various temperatures. (b) Relationships between dissolution time and dissolved weight of solute at 50℃, 18.0 MPa.

Linear relationships between the logarithms solubility and the logarithms density of $scCO_2$ were obtained at various temperatures when $p \geq 12.0$ MPa, as shown in Fig.S1(a). The solubility at 323.15 K and 333.15 K was higher than that at 313.15 K, which indicated that temperature played a dominant factor in solubility at high density.

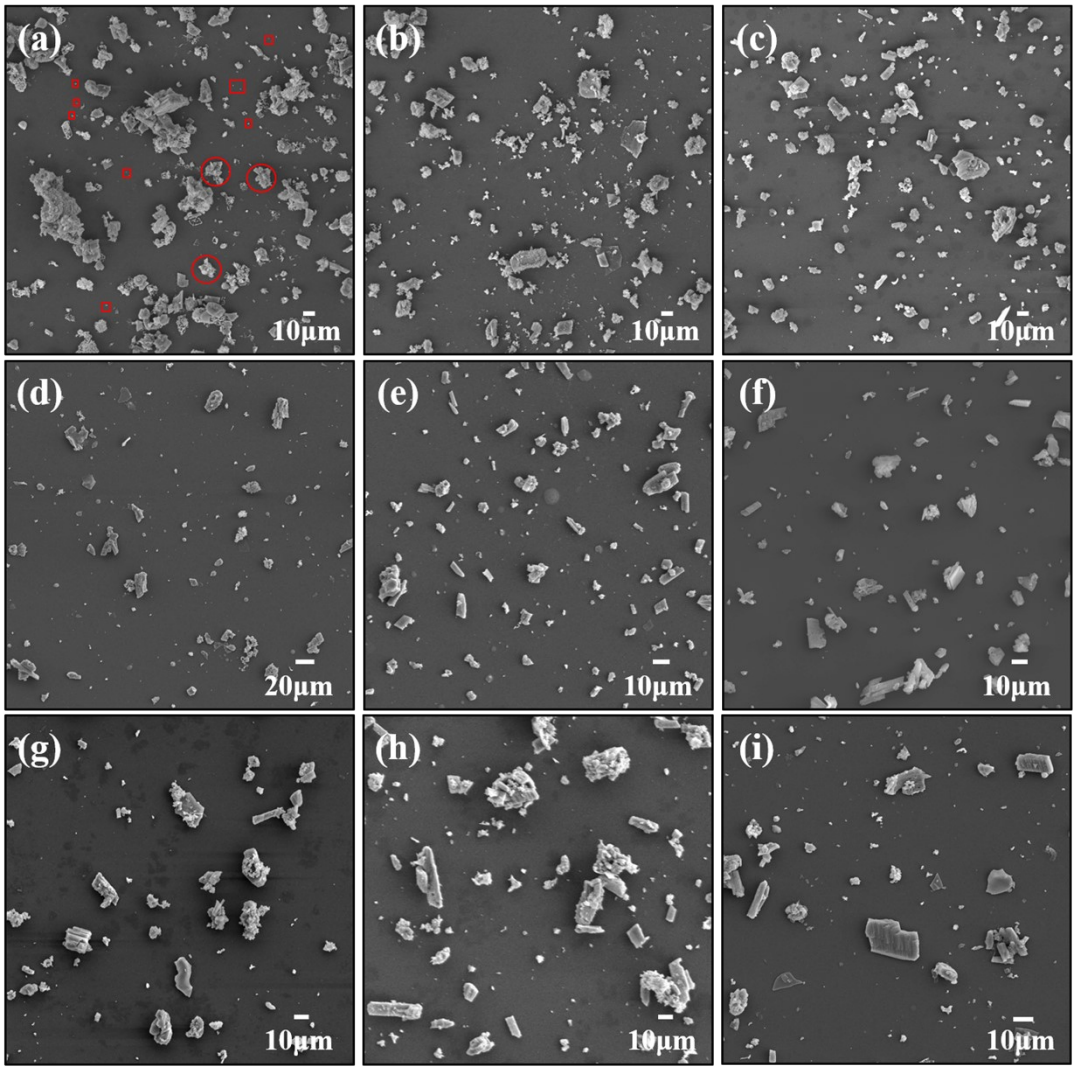

Fig.S2 SEM images of $MoO_2(acac)_2$ particles obtained by PI-SCPN process at p=20.0 MPa, various temperatures and supersaturation. (a) T=333.15 K, σ_c=12; (b) T=333.15 K, σ_c =8; (c) T=333.15 K, σ_c =5; (d) T=323.15 K, σ_c =12; (e) T=323.15 K, σ_c =8; (f) T=323.15 K, σ_c =5; (g) T=313.15 K, σ_c =12; (h) T=313.15 K, σ_c =8; (i) T=313.15 K, σ_c =5.

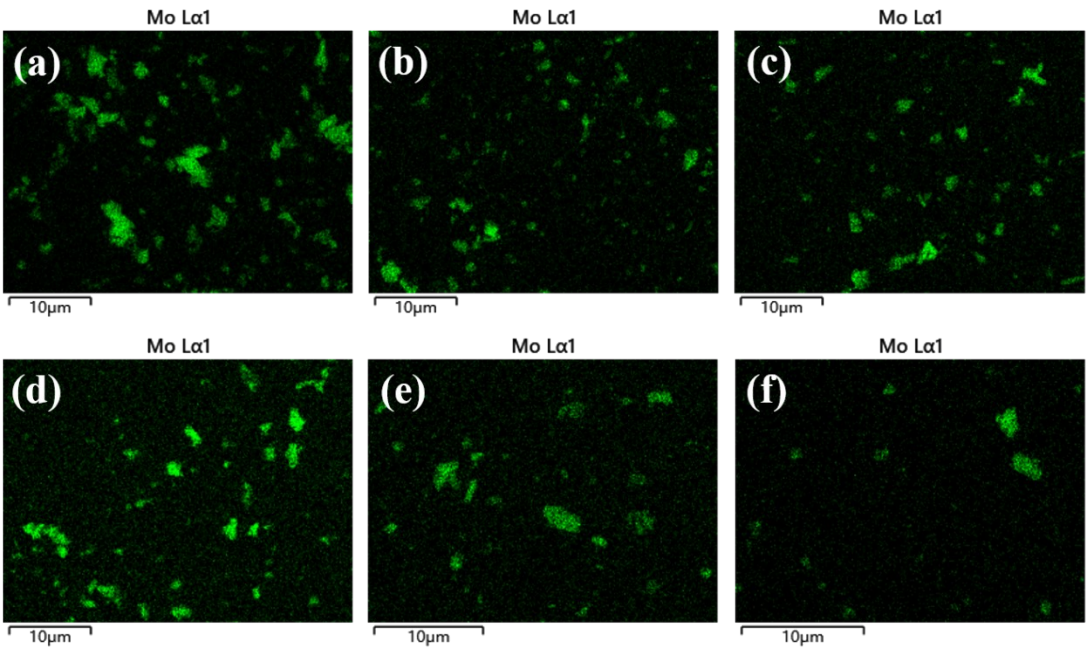

Fig. S3 EDS images of some samples (a) Sample 1, T=333.15 K, p=20.0 MPa, σ=12; (b) Sample 3, T=333.15 K, p=20.0 MPa, σ=5; (c) Sample 6, T=323.15 K, p=20.0 MPa, σ=5; (d) Sample 7, T=313.15 K, p=20.0 MPa, σ=12; (e) Sample 9, T=313.15 K, p=20.0 MPa, σ=5; (f) Sample 12, T=323.15 K, p=14.0 MPa, σ=5.

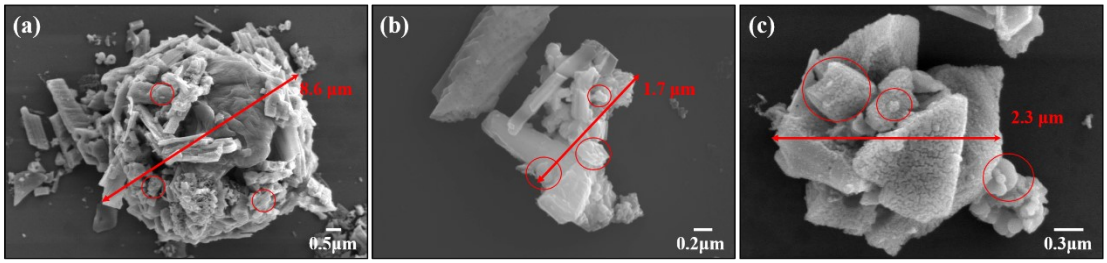

Fig. S4 SEM images of agglomerated particles at various operating conditions (a) T=333.15 K, p=20.0 MPa, σ=12; (b) T=323.15 K, p=20.0 MPa, σ=5; (c) T=313.15 K, p=20.0 MPa, σ=12.

In Fig. S4, the size of the agglomerated structure was significantly larger than that of a cluster. The red circle contained at least one cluster.

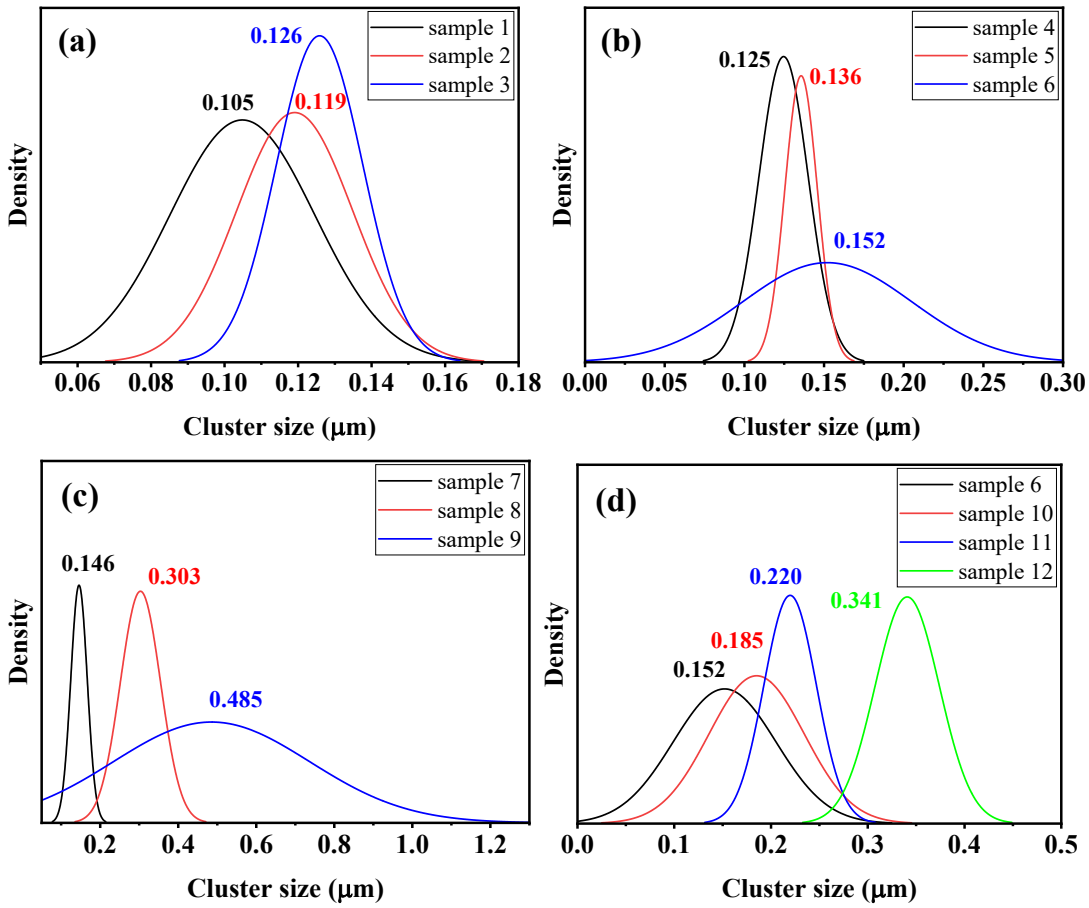

Fig. S5 Statistical distribution of cluster size *r* at various conditions. (a) samples 1, 2, and 3;(b) samples 4, 5, and 6;(c) samples 7, 8, and 9; (d) samples 6, 10, 11, and 12.

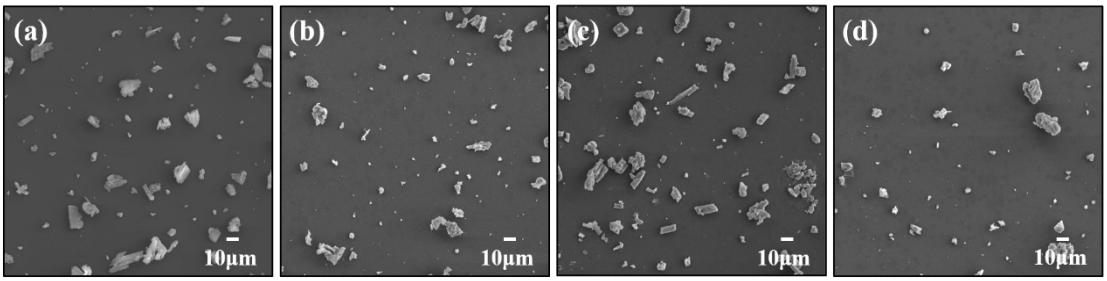

Fig. S6 SEM image of Cluster at T=323.15 K, σ_c =5 and various pressure; (a) p=20.0 MPa; (b) p=18.0 MPa; (c) p=16.0 MPa; (d) p=14.0 MPa.