

**Electronic Supplementary Material**  
**Reduction kinetics of SrFeO<sub>3-δ</sub>/CaO·MnO nanocomposite**  
**as effective oxygen carrier for chemical looping partial**  
**oxidation of methane**

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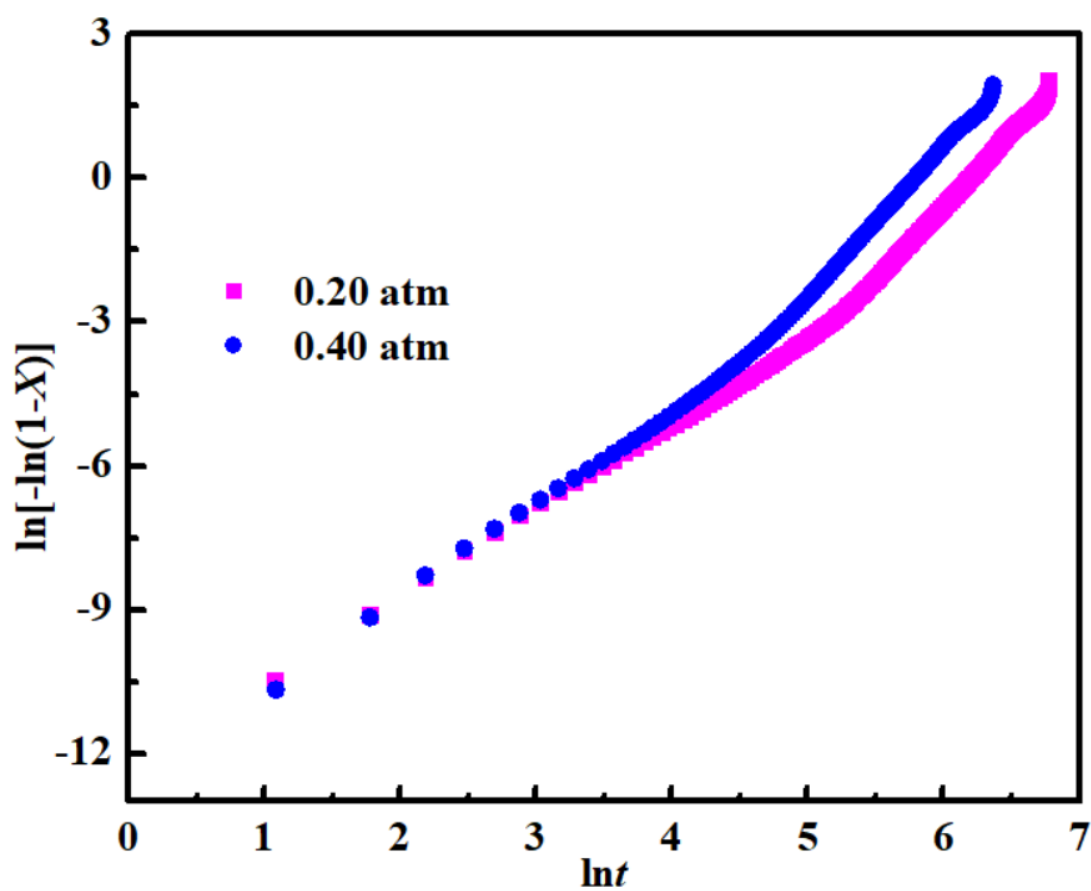
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**Table S1.** Solid-state rate and integral expressions for different reaction models [1]

Model / Mechanism	Differential form $f(X) = 1/k dX/dt$	Integral form $g(X) = kt$
<b>Nucleation models</b>		
Power law (P2)	$2X^{1/2}$	$X^{1/2}$
Power law (P3)	$3X^{2/3}$	$X^{1/3}$
Power law (P4)	$4X^{3/4}$	$X^{1/4}$
Avrami-Erofeyev (A2)	$2(1-X)[- \ln(1-X)]^{1/2}$	$[- \ln(1-X)]^{1/2}$
Avrami-Erofeyev (A3)	$3(1-X)[- \ln(1-X)]^{2/3}$	$[- \ln(1-X)]^{1/3}$
Avrami-Erofeyev (A4)	$4(1-X)[- \ln(1-X)]^{3/4}$	$[- \ln(1-X)]^{1/4}$
Prout-Tompkins (B1)	$X(1-X)$	$\ln[X/(1-X)] + c^n$
<b>Geometrical contraction models</b>		
Contracting area (R2)	$2(1-X)^{1/2}$	$1 - (1-X)^{1/2}$
Contracting area (R3)	$3(1-X)^{2/3}$	$1 - (1-X)^{1/3}$
<b>Diffusion models</b>		
1-D diffusion (D1)	$1/(2X)$	$X^2$
2-D diffusion (D2)	$-[1/\ln(1-X)]$	$((1-X)\ln(1-X)) + X$
3-D diffusion-Jander (D3)	$[3(1-X)^{2/3}]/[2(1-(1-X)^{1/3})]$	$(1-(1-X)^{1/3})^2$
Ginstling-Brounshtein (D4)	$3/[2((1-X)^{-1/3} - 1)]$	$1 - (2/3)X - (1-X)^{2/3}$
<b>Reaction-order models</b>		
Zero-order (F0/R1)	1	$X$
First-order (F1)	$1-X$	$-\ln(1-X)$
Second-order (F2)	$(1-X)^2$	$[1/(1-X)] - 1$
Third-order (F3)	$(1-X)^3$	$(1/2)[(1-X)^{-2} - 1]$

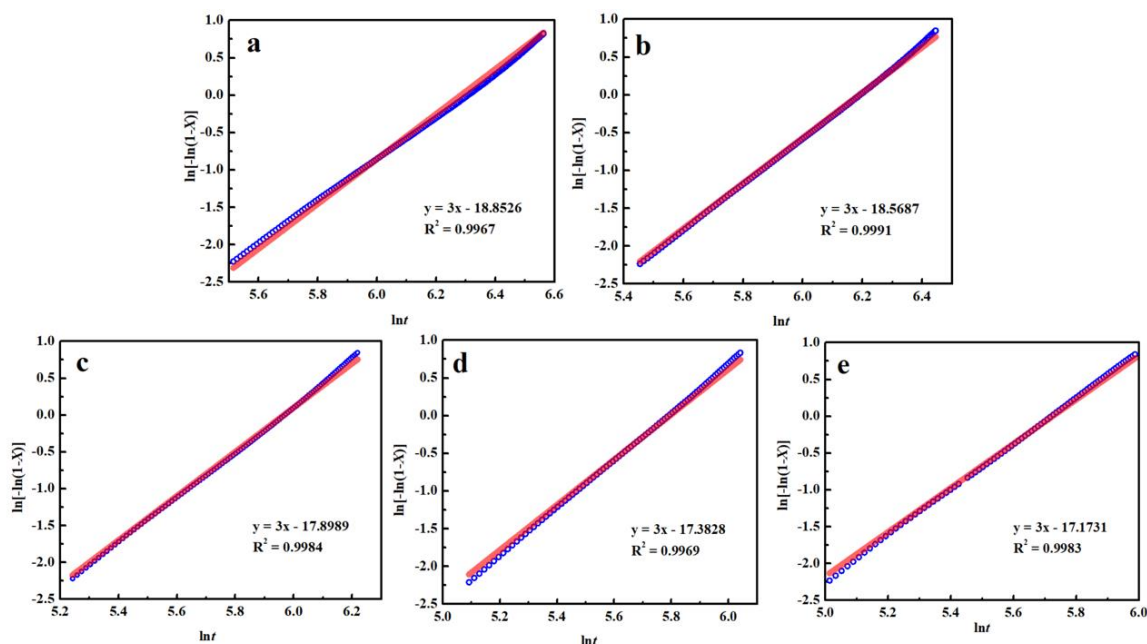
**Table S2.** Comparison of the activation energy reported in the literature

Redox materials	Temperature range	Experimental method	$E_a$ (kJ/mol)	Ref.
10%Co/mesoporous alumina	973–1073 K	Isothermal TCD	43.48	[2]
$\text{Sr}_{2.45}\text{La}_{0.55}\text{FeCoO}_{7-\delta}$	1073–1173 K	Isothermal GC	58.3	[3]
NiO/MgAl <sub>2</sub> O <sub>4</sub>	1073–1273 K	Isothermal TGA	114	[4]
$\text{SrFeO}_{3-\delta}\text{-CaO}\cdot\text{MnO}$	1123~1223 K	Isothermal TGA	59.8	This work



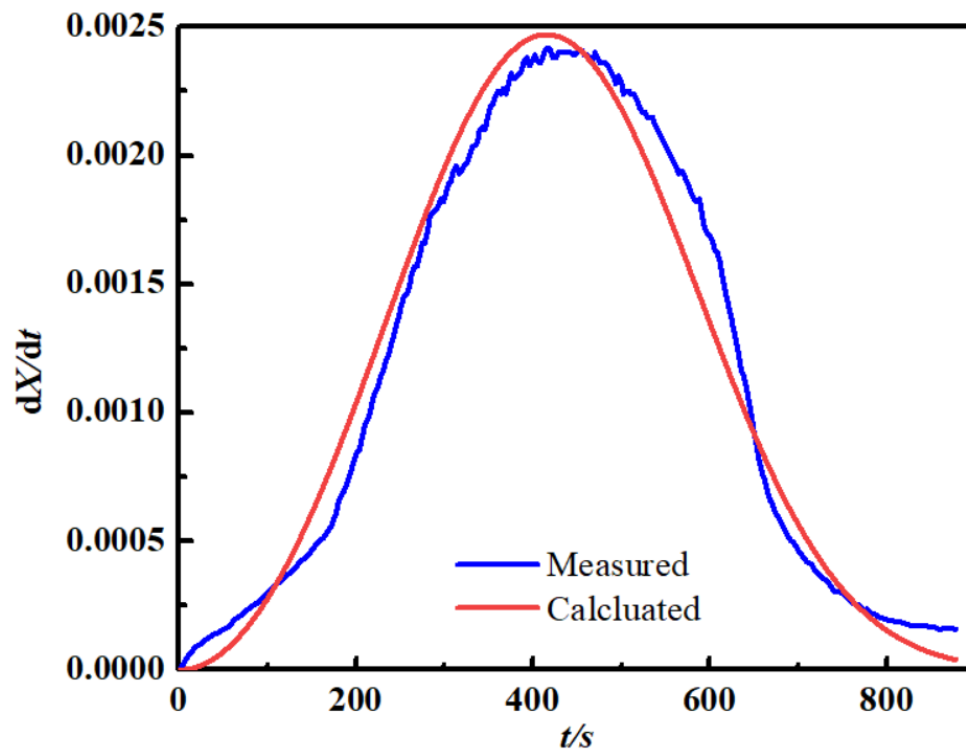
**Fig. S1.** The plots of  $\ln[-\ln(1-X)]$  as function of time  $t$  for two methane pressures,

Reaction conditions:  $m_{\text{SF-CM}} = 1$  g,  $T = 900$  °C,  $F = 110$  STP mL/min,  $P = 1$  atm.

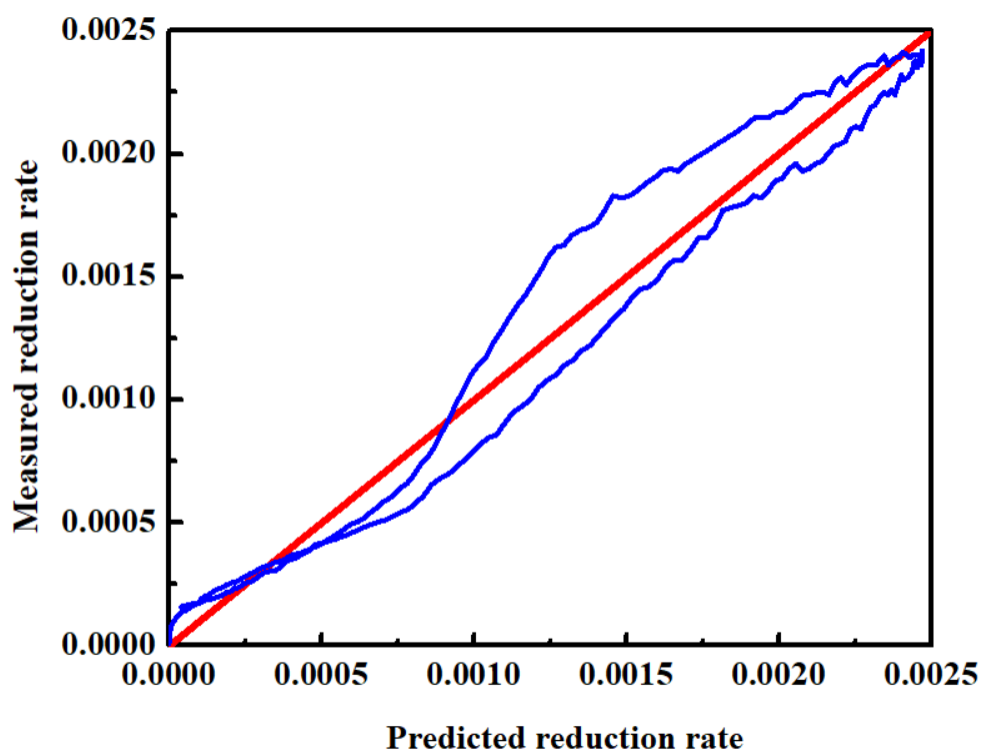


**Fig. S2.** The plots of  $\ln[-\ln(1-X)]$  vs.  $\ln t$  for five methane pressures: (a) 0.15 atm, (b) 0.20 atm, (c) 0.30 atm, (d) 0.40 atm, (e) 0.50 atm. Reaction conditions:  $m_{\text{SF-CM}} = 1$  g,

$T = 900$  °C,  $F=110$  STP mL/min,  $P=1$  atm.



**Fig. S3.** The predicted and measured reduction rates for a methane partial pressure of 0.20 atm. Reaction conditions:  $m_{\text{SF-CM}} = 1$  g,  $T = 900$  °C,  $F = 110$  STP mL/min,  $P = 1$  atm.



**Fig. S4.** The Q-Q plot for a methane partial pressure of 0.20 atm. Reaction conditions:

$$m_{\text{SF-CM}} = 1 \text{ g}, T = 900 \text{ }^{\circ}\text{C}, F = 110 \text{ STP mL/min}, P = 1 \text{ atm.}$$

## References

1. Khawam A, Flanagan DR. Solid-state kinetic models: basics and mathematical fundamentals, *The Journal of Physical Chemistry B*, 2006, 110(35): 17315-28
2. Tran NT, Van Le Q, Van Cuong N, Nguyen TD, Huy Phuc NH, Phuong PTT, Monir MU, Aziz AA, Truong QD, Abidin SZ, Nanda S, Vo DVN. La-doped cobalt supported on mesoporous alumina catalysts for improved methane dry reforming and coke

mitigation. Journal of the Energy Institute, 2020, 93(4):1571-1580

3. Kagomiya I, Suzumura M, Kakimoto Ki, Ohsato H. Influence of Layered Perovskite Structure on Oxygen Permeability of Sr–La–Fe–Co Oxide. Journal of the Physical Society of Japan, 2010,79: 109-112

4. Zafar Q, Abad A, Mattisson T, Gevert B. Reaction Kinetics of Freeze-Granulated NiO/MgAl<sub>2</sub>O<sub>4</sub> Oxygen Carrier Particles for Chemical-Looping Combustion. Energy & Fuels, 2007, 21(2): 610-618