# Paper presentation

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

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Article

# Microdroplet Cascade Catalysis for Highly Selective Production of Propylene Glycol under Ambient Conditions

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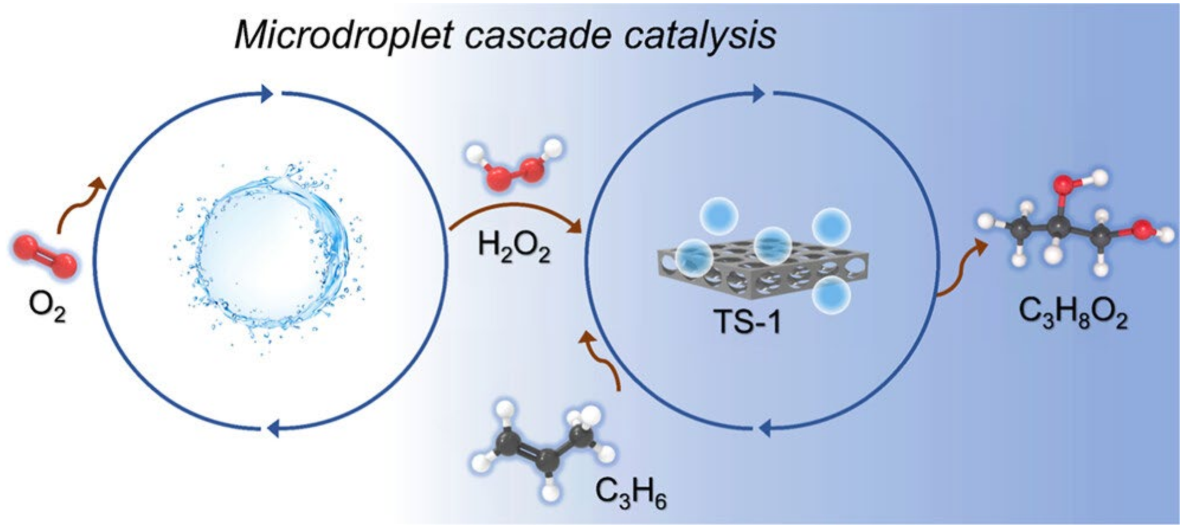
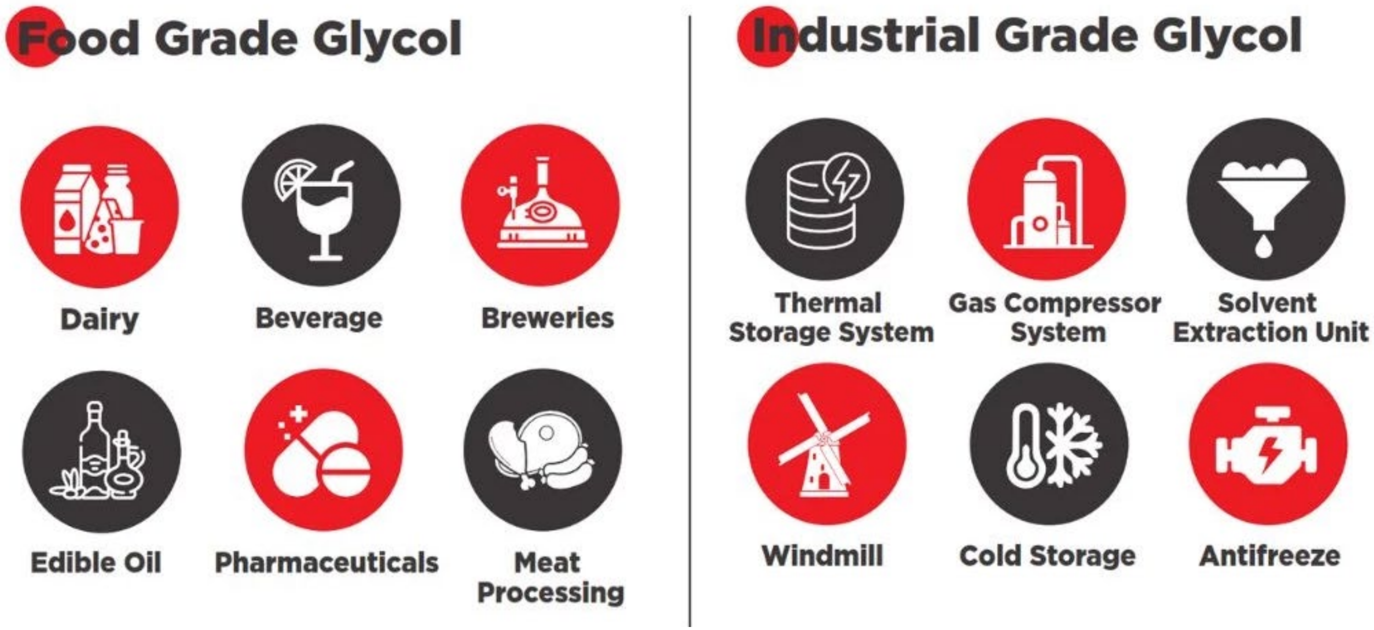



**21-06-2025**

## Uses of Propylene glycol




Drawbacks during production:

- High temperature (150°C to 250°C)
- Low selectivity, by-product formation due to overoxidation

https://www.chemtexltd.com/propylene-glycol-has-many-uses-beyond-just-being-an-antifreeze-discover-some-of-them-here/

*Journal of the American Chemical Society* > Vol 147/Issue 13 > Article
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ARTICLE | March 24, 2025

# Charged Water Microdroplets Enable Dissociation of Surrounding Dioxygen

Jian Zhou, Qing Wang, Gongkui Cheng, Wei Shen, Richard N. Zare*, and Xiaoyan Sun*

*Journal of the American Chemical Society* > Vol 144/Issue 8 > Article
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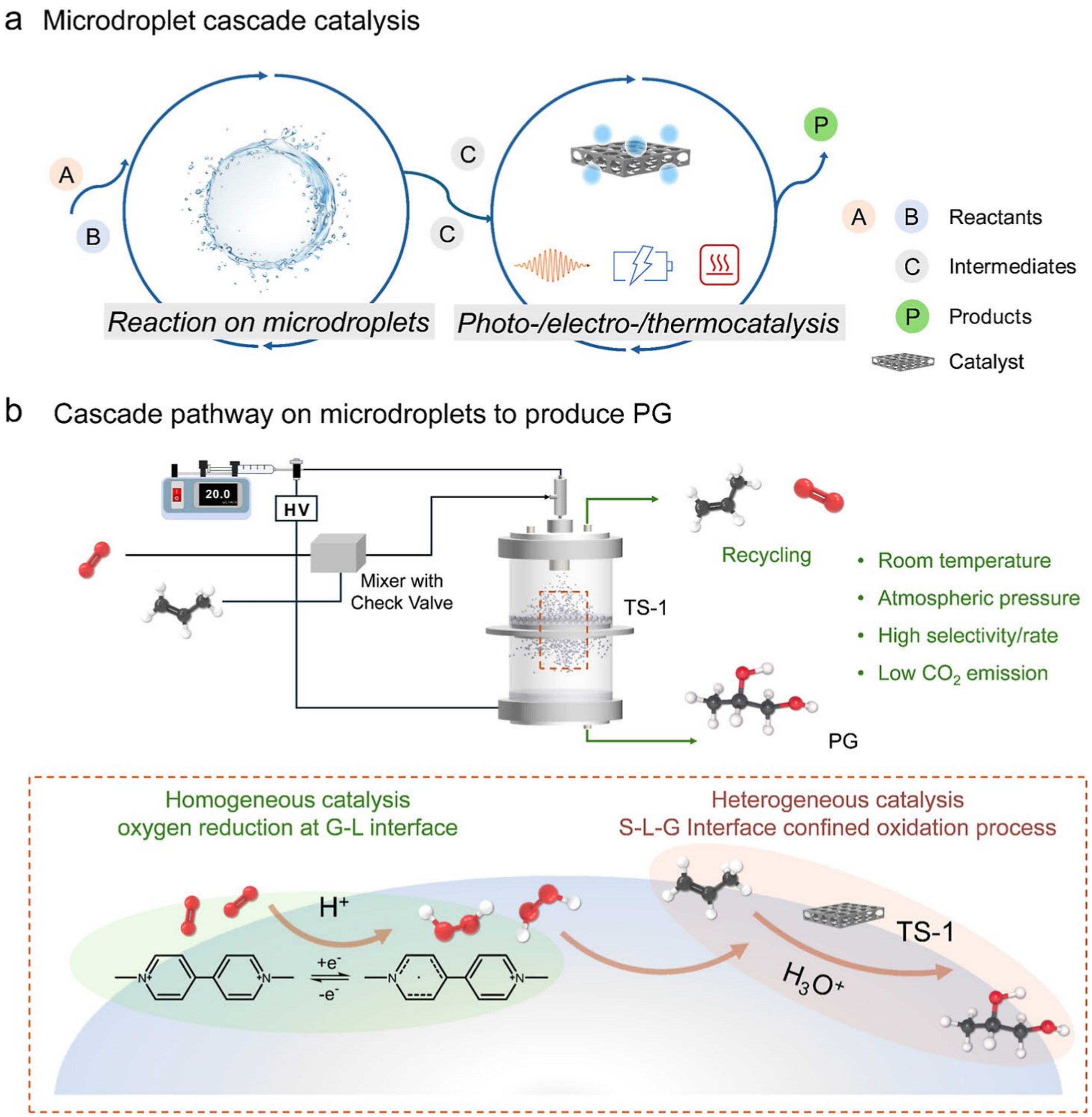
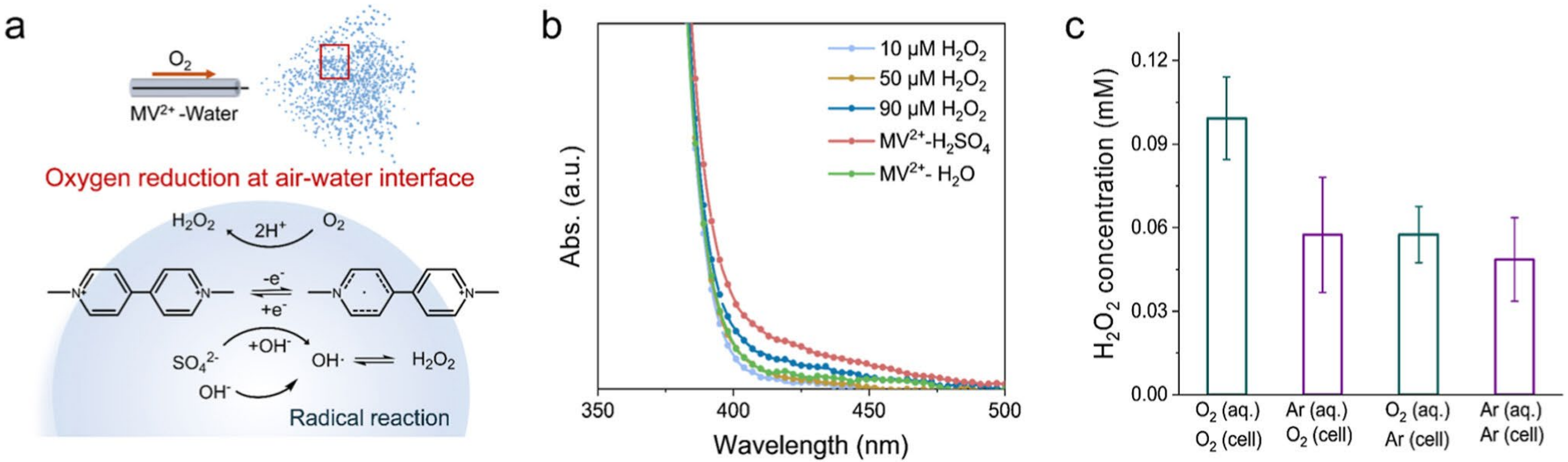
ARTICLE | February 15, 2022

# Spontaneous Reduction-Induced Degradation of Viologen Compounds in Water Microdroplets and Its Inhibition by Host–Guest Complexation

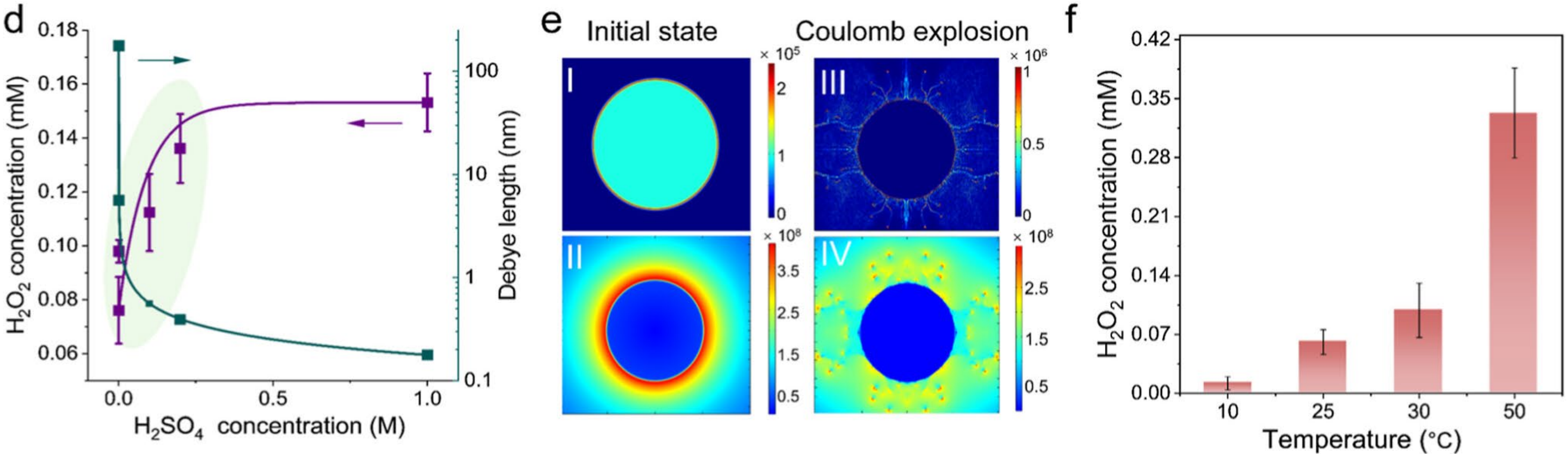
Chu Gong, Danyang Li, Xilai Li, Dongmei Zhang, Dong Xing, Lingling Zhao, Xu Yuan, and Xinxing Zhang*




TS-1 → Titanium Silicalite-1




"Cell" denotes the sheath gas and reaction chamber having the same gas, while "aq." indicates gas present in the aqueous phase.


d
0.18
0.16
0.14
0.12
0.10
0.08
0.06
H2O2 concentration (mM)
100
10
1
0.1
Debye length (nm)
0.0
0.5
1.0
H2SO4 concentration (M)
e
Initial state
Coulomb explosion
I
II
III
IV
× 10^5
× 10^6
× 10^8
× 10^8
f
0.42
0.35
0.28
0.21
0.14
0.07
0.00
H2O2 concentration (mM)
10
25
30
50
Temperature (°C)

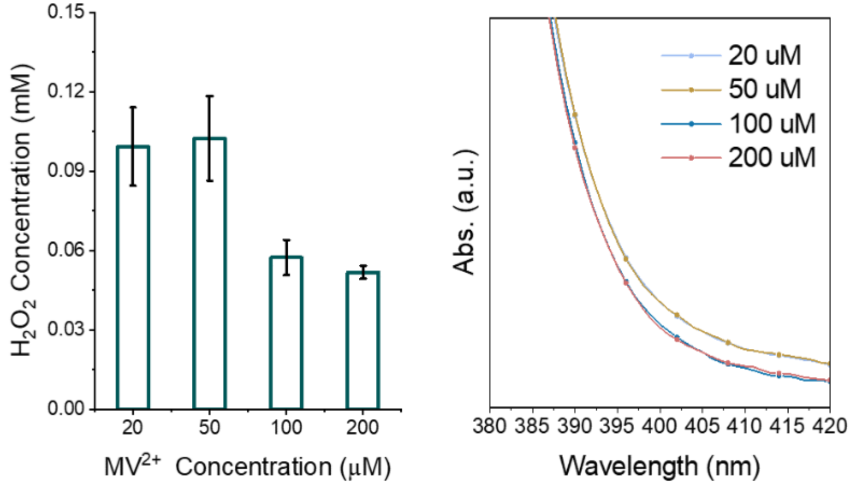



**Figure S4.** The $H_2O_2$ concentration and absorption spectra of samples under different $MV^{2+}$ concentrations.

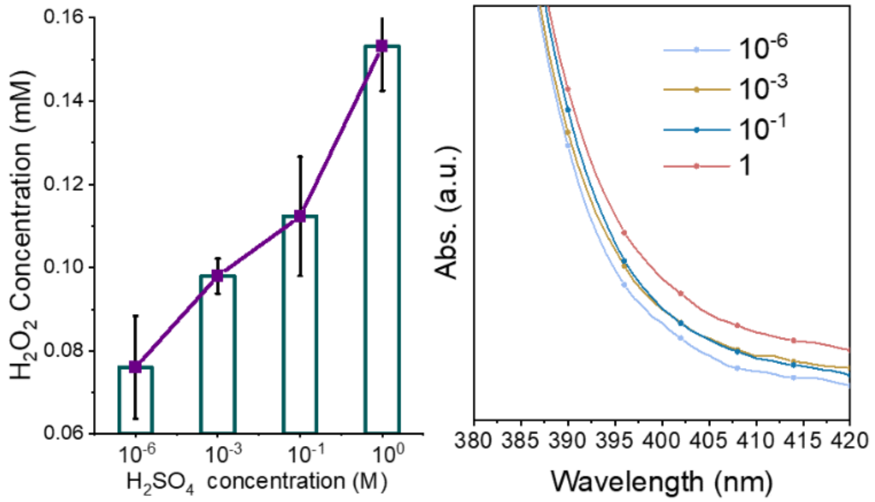



**Figure S5.** The $H_2O_2$ concentration and absorption spectra of samples under different $H_2SO_4$ concentrations.

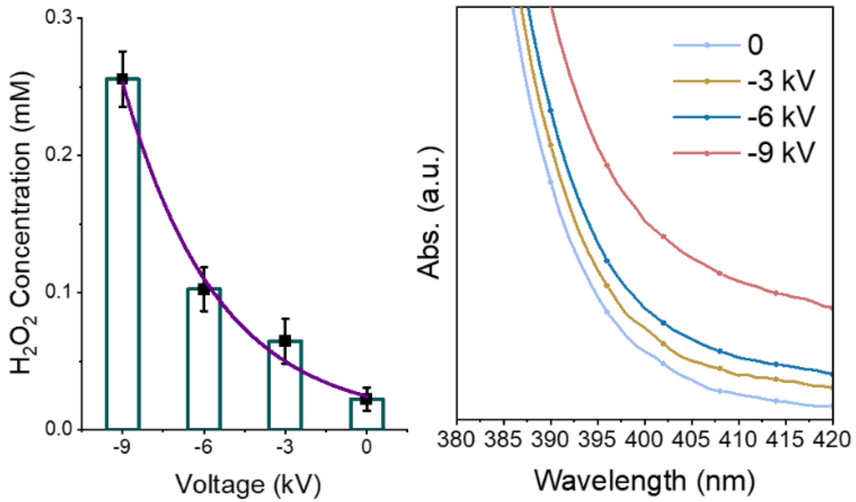
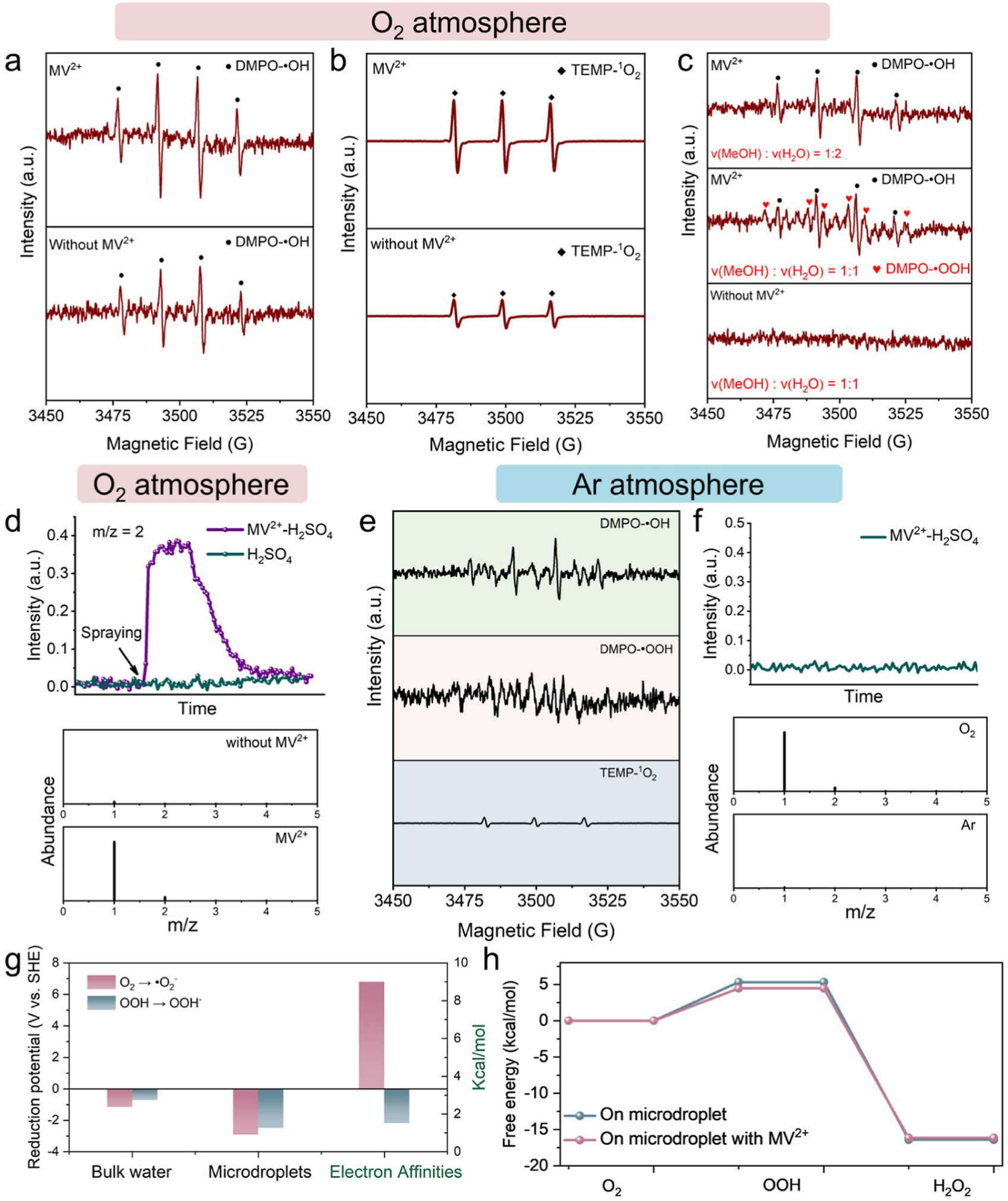
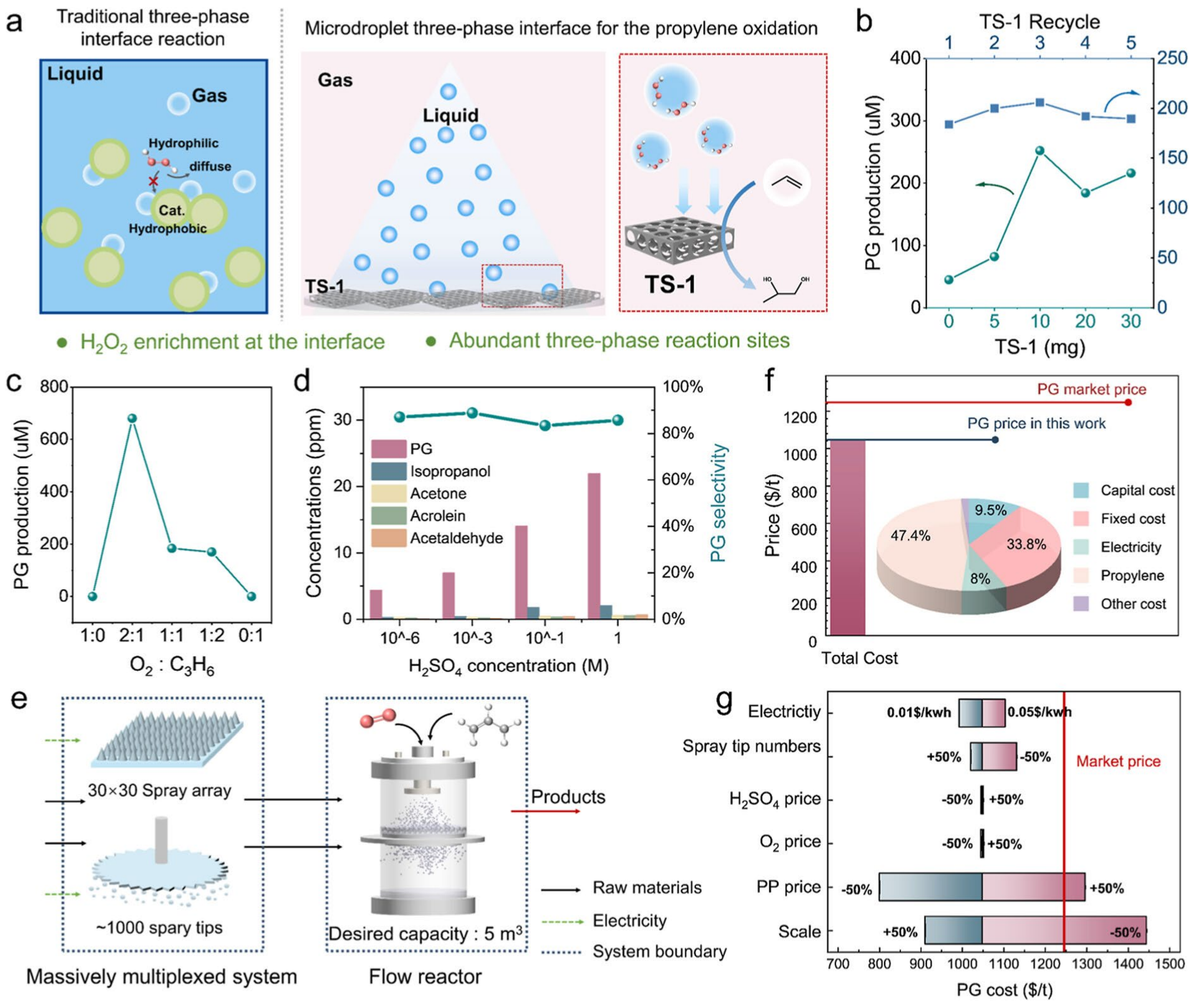



**Figure S7.** The $H_2O_2$ concentration and absorption spectra of samples under different applied voltages.



O2 atmosphere
a
MV2+
• DMPO-•OH
Without MV2+
Intensity (a.u.)
3450 3475 3500 3525 3550
Magnetic Field (G)
b
MV2+
◆ TEMP-1O2
without MV2+
c
v(MeOH) : v(H2O) = 1:2
v(MeOH) : v(H2O) = 1:1
♥ DMPO-•OOH
O2 atmosphere
d
m/z = 2
MV2+-H2SO4
H2SO4
Spraying
Time
Abundance
m/z
Ar atmosphere
e
DMPO-•OH
DMPO-•OOH
TEMP-1O2
f
O2
Ar
g
O2 → •O2-
OOH → OOH-
Reduction potential (V vs. SHE)
Kcal/mol
Bulk water
Microdroplets
Electron Affinities
h
Free energy (kcal/mol)
On microdroplet
On microdroplet with MV2+
O2
OOH
H2O2


a
Traditional three-phase interface reaction
Liquid
Gas
Hydrophilic
diffuse
Cat.
Hydrophobic
Microdroplet three-phase interface for the propylene oxidation
Gas
Liquid
TS-1
TS-1
● $H_2O_2$ enrichment at the interface
● Abundant three-phase reaction sites
b
TS-1 Recycle
PG production (uM)
TS-1 (mg)
c
PG production (uM)
$O_2 : C_3H_6$
d
Concentrations (ppm)
PG selectivity
PG
Isopropanol
Acetone
Acrolein
Acetaldehyde
$H_2SO_4$ concentration (M)
f
PG market price
PG price in this work
Price ($/t)
Total Cost
Capital cost
Fixed cost
Electricity
Propylene
Other cost
9.5%
33.8%
8%
47.4%
e
30×30 Spray array
~1000 spary tips
Products
Desired capacity : 5 m³
Raw materials
Electricity
System boundary
Massively multiplexed system
Flow reactor
g
Electrictiy
Spray tip numbers
$H_2SO_4$ price
$O_2$ price
PP price
Scale
0.01$/kwh
0.05$/kwh
Market price
PG cost ($/t)

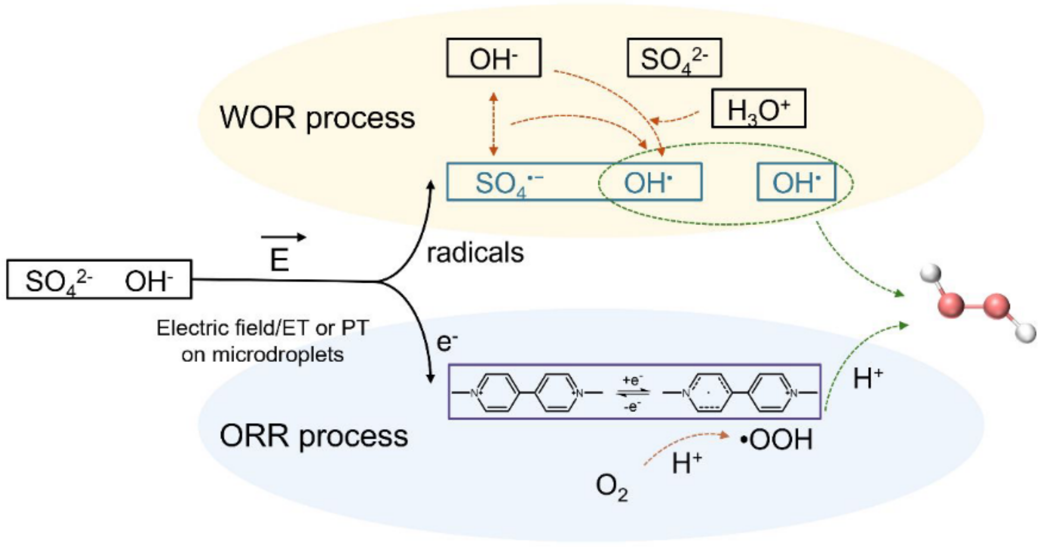



**Figure S15.** Proposed overall reaction mechanisms for $H_2O_2$ production catalyzed by a $MV^{2+}$ molecular catalyst in microdroplets.

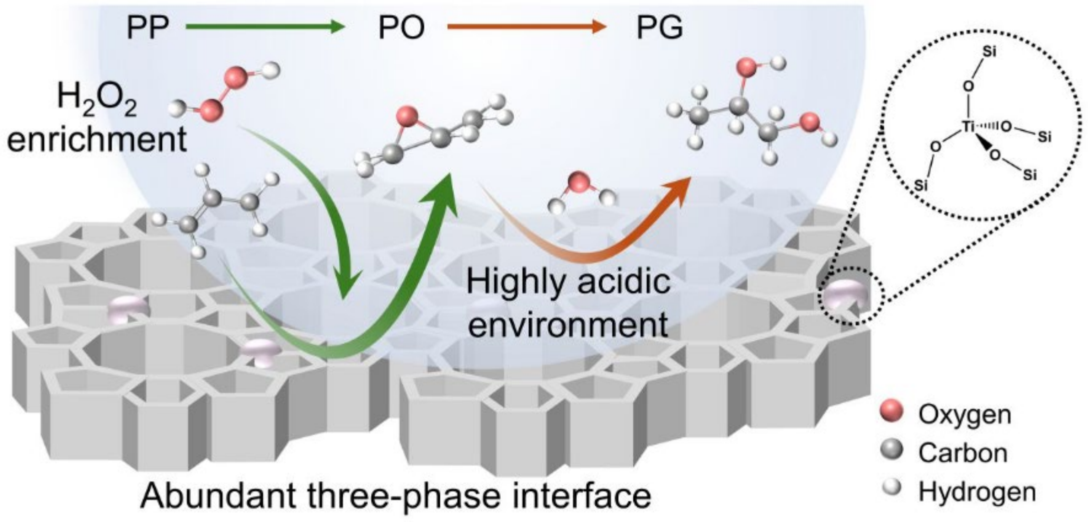
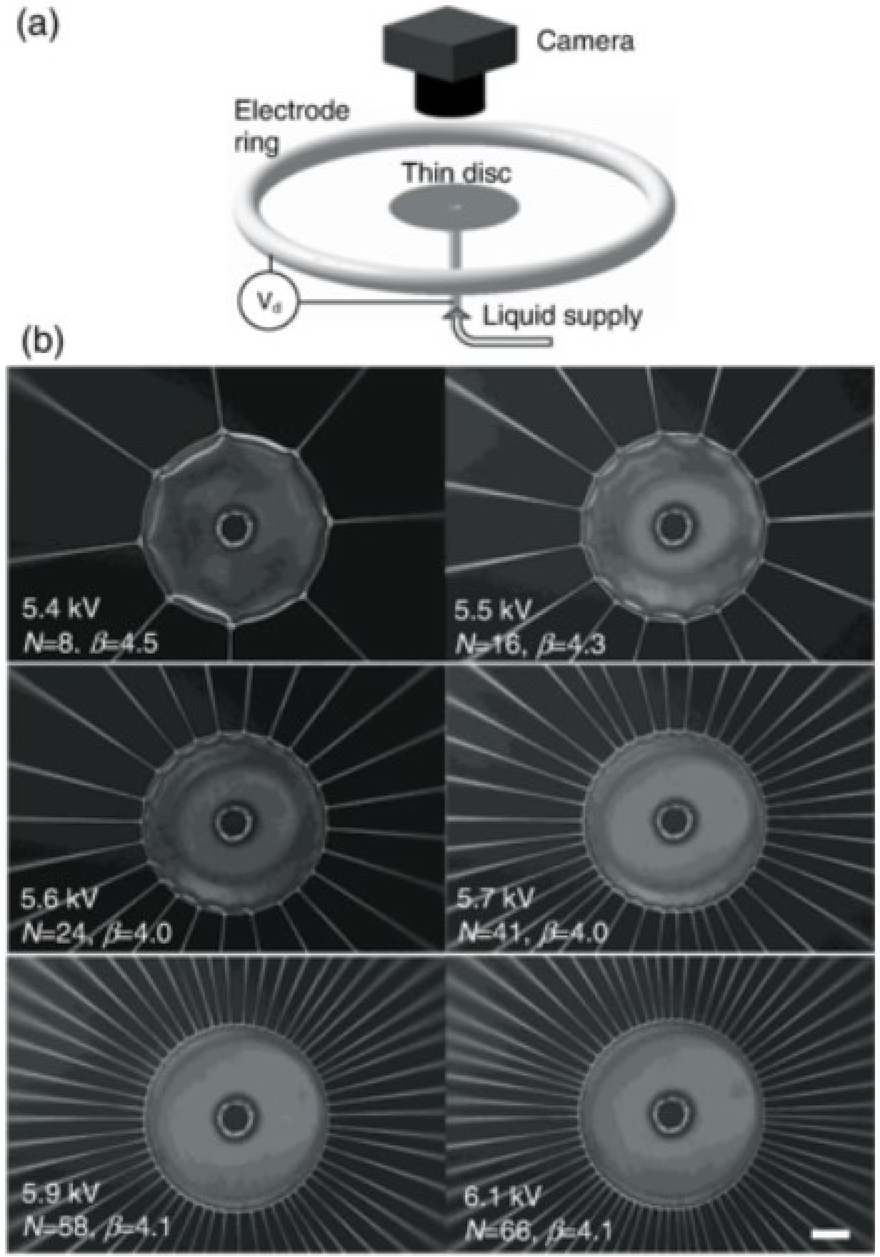
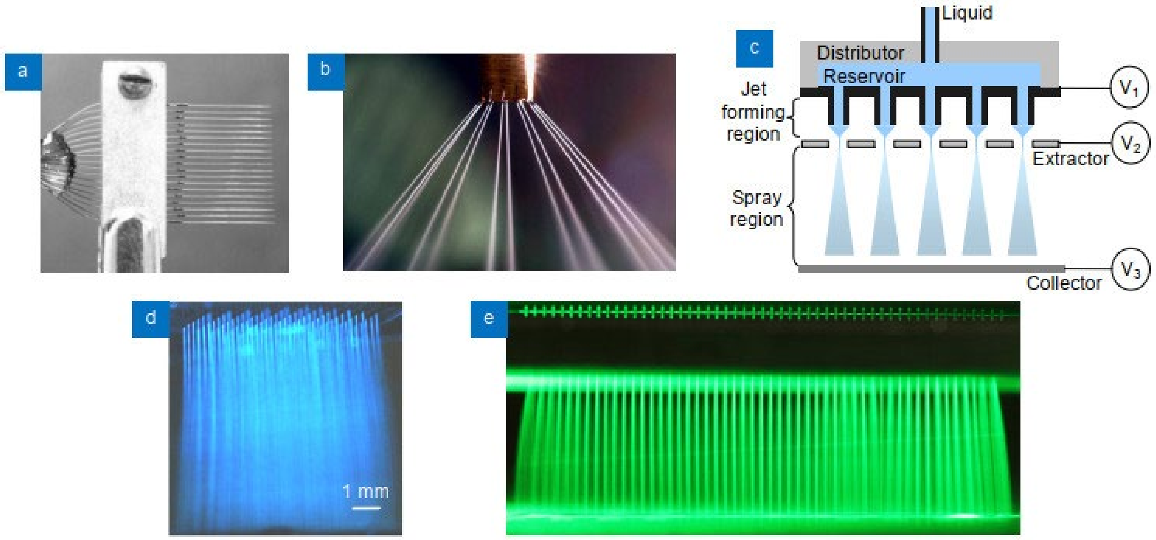



**Figure S16.** Proposed reaction mechanism in the cascade catalysis system.

**Conclusion**:

- Propylene glycol is produced from Propylene and $O_2$ using "microdroplet cascade catalysis". Use of Methyl Viologen enhances the electron transfer on the droplet  surface, hence improves the efficiency of the ORR reaction.
- Use of TS 1 catalyst triggers the efficiency of the oxidation of propylene oxide at the Solid-liquid-gas interface.


(a)
Camera
Electrode ring
Thin disc
$V_d$
Liquid supply
(b)
5.4 kV
N=8, β=4.5
5.5 kV
N=16, β=4.3
5.6 kV
N=24, β=4.0
5.7 kV
N=41, β=4.0
5.9 kV
N=58, β=4.1
6.1 kV
N=66, β=4.1


a
b
c
Liquid
Distributor
Reservoir
$V_1$
Jet forming region
$V_2$
Extractor
Spray region
$V_3$
Collector
d
1 mm
e