Nanomaterials Enabled Smart Systems

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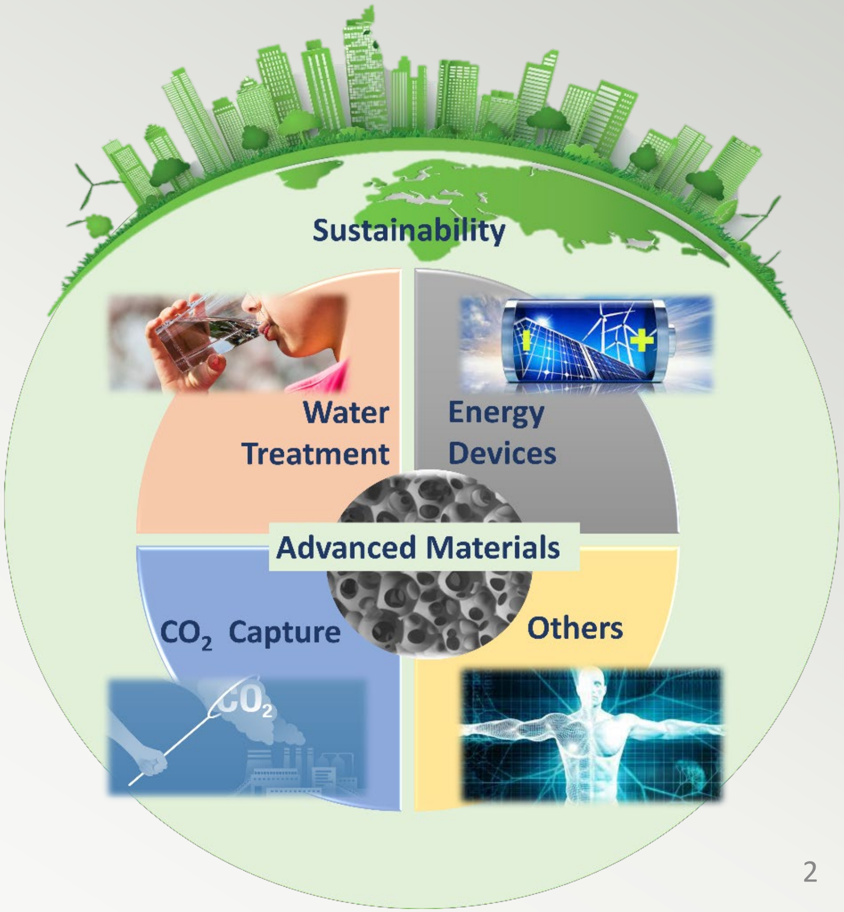
April 30th, 2024

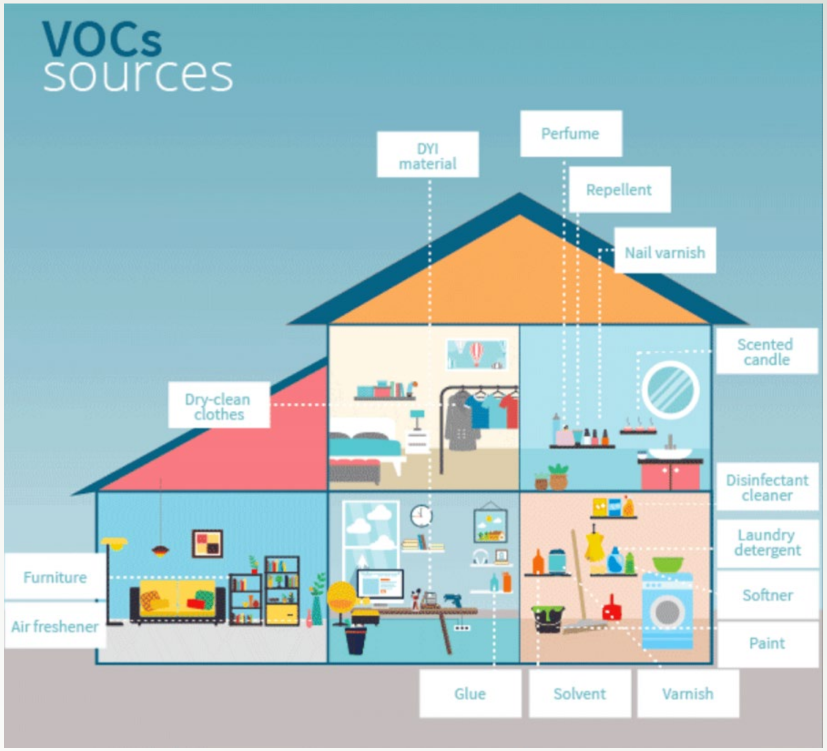
Overview

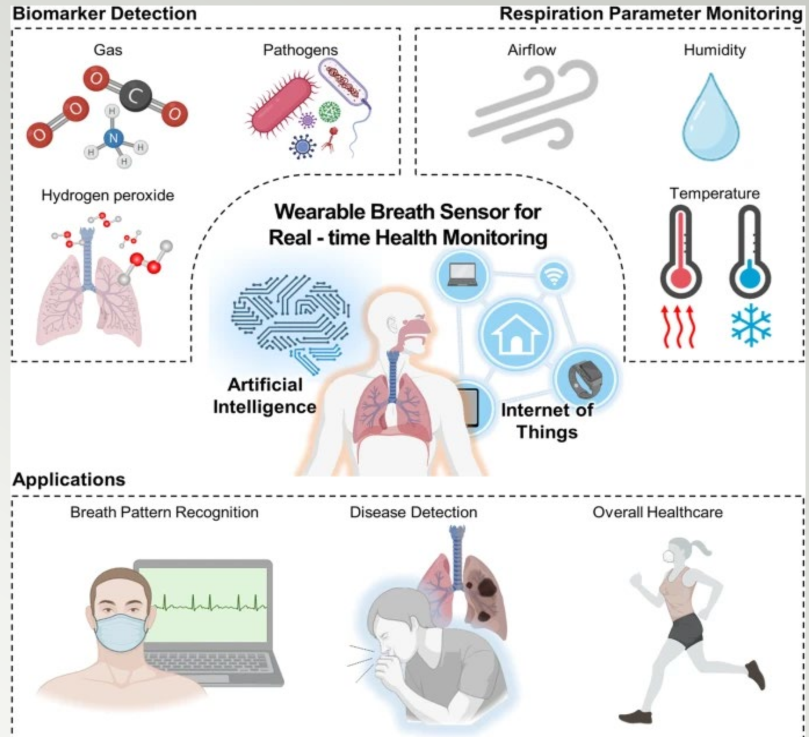
Nanomaterials Enabled Smart Systems

1. For public health
2. for water treatment
3. for energy devices



Hazardous materials: solid, liquid & gas





Indoor hazard

- Formaldehyde (CH2O)
- Long-term health effects & cause cancer

Biomarkers for specific diseases

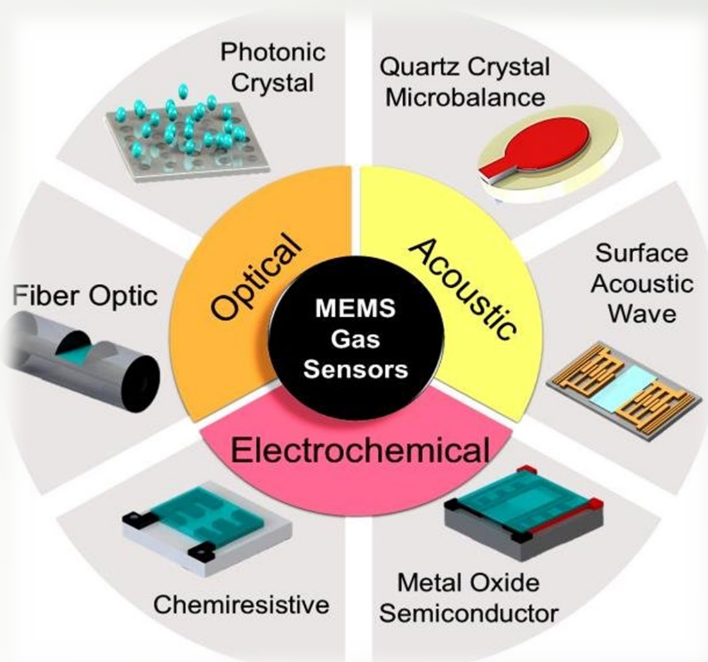
- Cyclohexane and benzene levels in breath: mycobacterium tuberculosis (M. tb)

https://www.airmasters.ca/2018/04/01/volatile-organic-compounds/

D. Kim, et. al, communications materials,5,41, 2024

Existing sensors

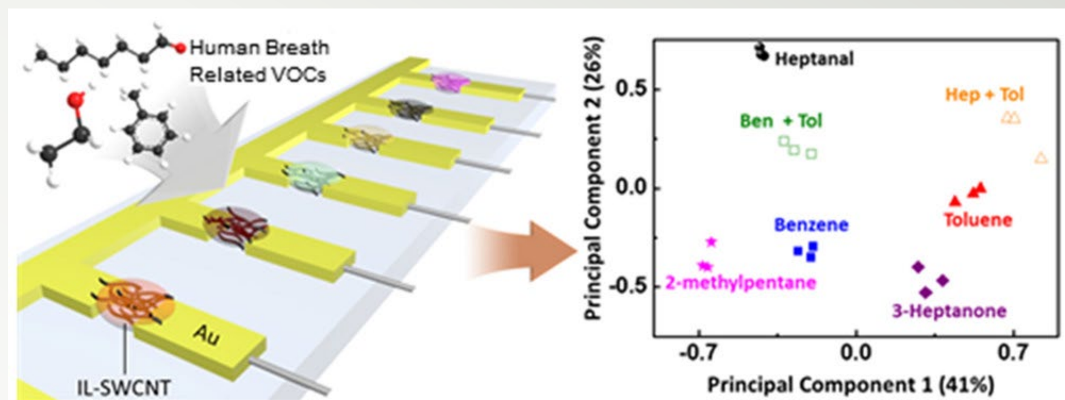
Sensors



Volatile organic compounds (VOC)

Electrochemical sensors:

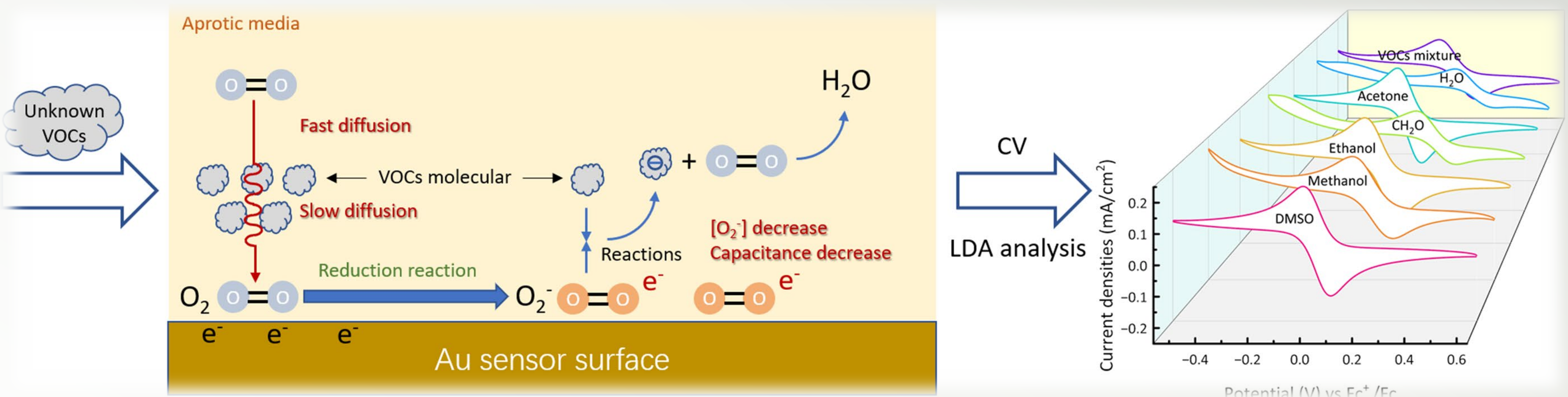
- **Advantages:** quantification at ppm level with low-power, high resolution, better repeatability
- **Disadvantages:** cross-sensitivity, narrow working temperature, difficulties in determining baseline



M. Asri, et. al, IEEE Sensors Journal, 99, 1, 2021
C. Park et. al, ACS sensors, 3, 11, 2432,2018

New approach:
Species-selective detection of VOC

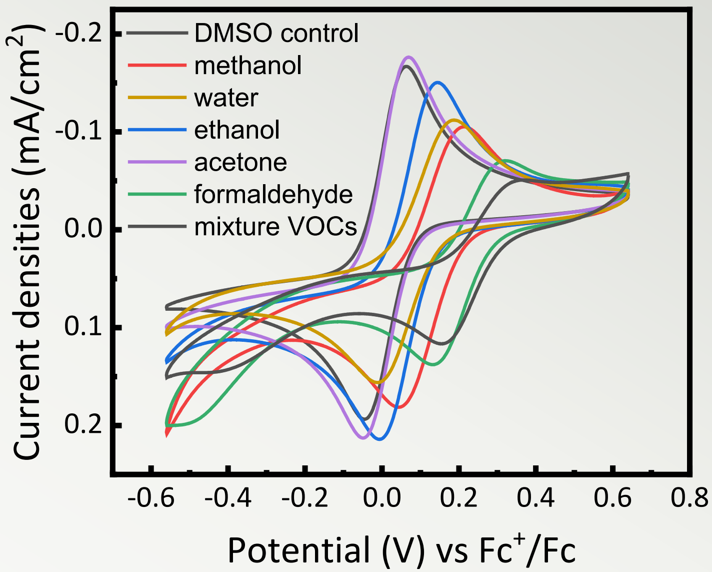
VOC detection & classification
- Methanol
- Ethanol
- Acetone
- Formaldehyde
- **And their mixer**

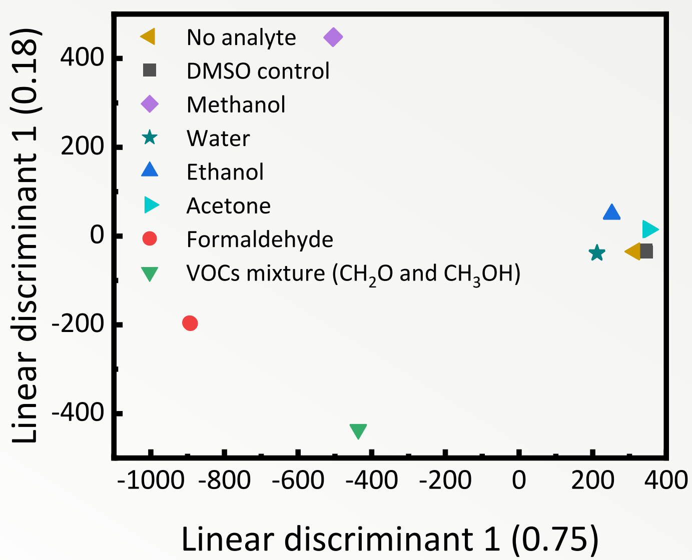


1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide [C4mpy] [NTf2]
dimethyl sulfoxide (DMSO)

X. Huang, et. al, P. Dong*, ACS Sensor, 2023, 8, 3389−3399

Machine learning approach:
Linear discriminant analysis (LDA)





Voltammogram

Feature extraction

Shape features

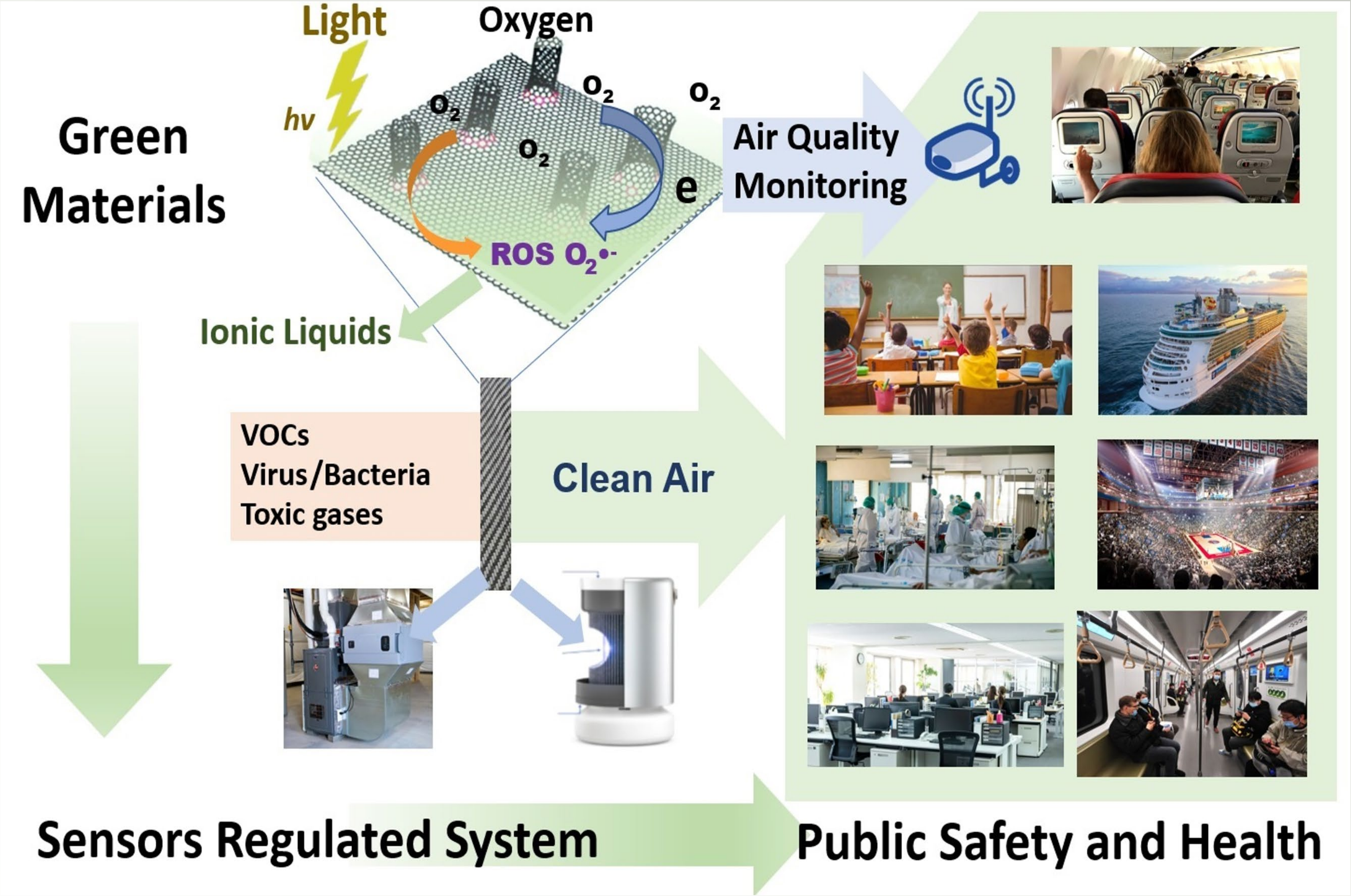
1. Curve fitting
2. Left and right endpoints

Redox peaks features

1. Potential
2. Height
3. Area

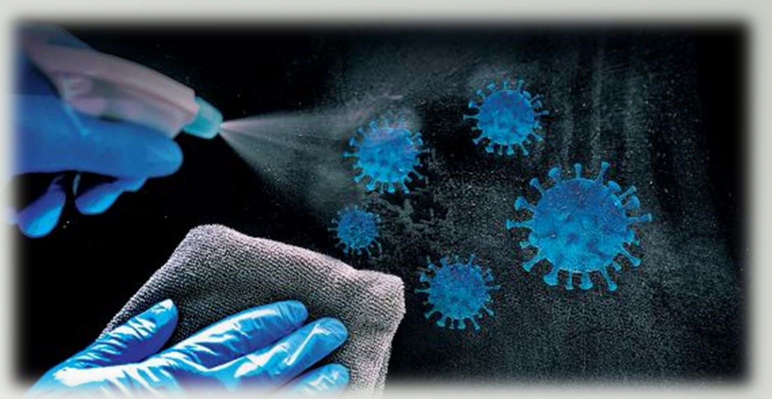
Linear Discriminant Analysis

Smart system for Hazard Detection & Disinfection



Current solution for disinfectant

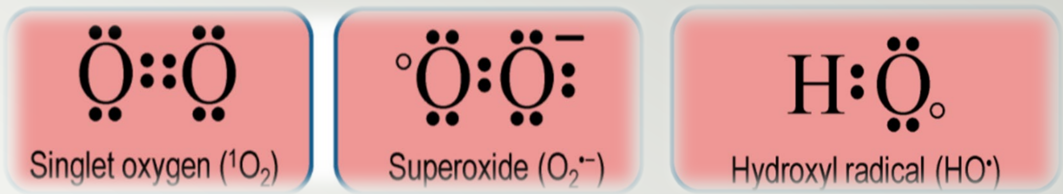
- Common disinfectant: ethanol, Isopropanol, hydrogen peroxide, phenol, lactic acid, chlorine dioxide, etc.
- Cost: $0.12 – $0.75 per sq. ft. or $85 - $125 per hour
- **Challenge:** evaporation and degradation, Cumulative consumption and labor work
- Demand for new disinfection technology with features in high efficiency, low-cost and reusable



https://www.thejanitorialstore.com/public/Coronavirus-2019-COVID19-Pandemic-Information-2265.cfm
https://www.cmmonline.com/articles/disinfection-done-right
https://news.psu.edu/story/619489/2020/05/11/research/researcher-explores-disinfectant-strength-contact-time-against

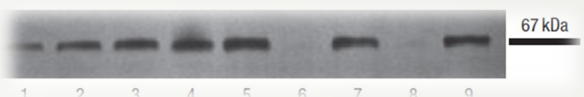
Reactive Oxygen Species (ROS)

ROS

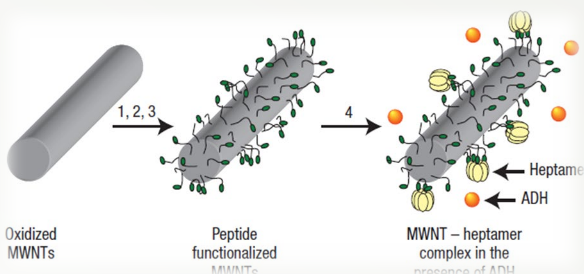


Applications

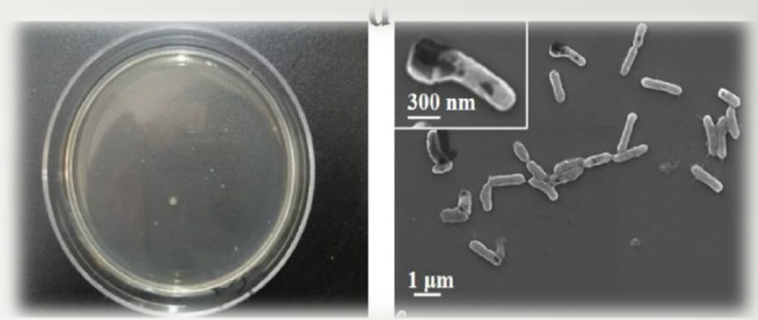
a. Self-cleaning membrane



b. Protein selectively deactivations



c. Bacteria disinfection

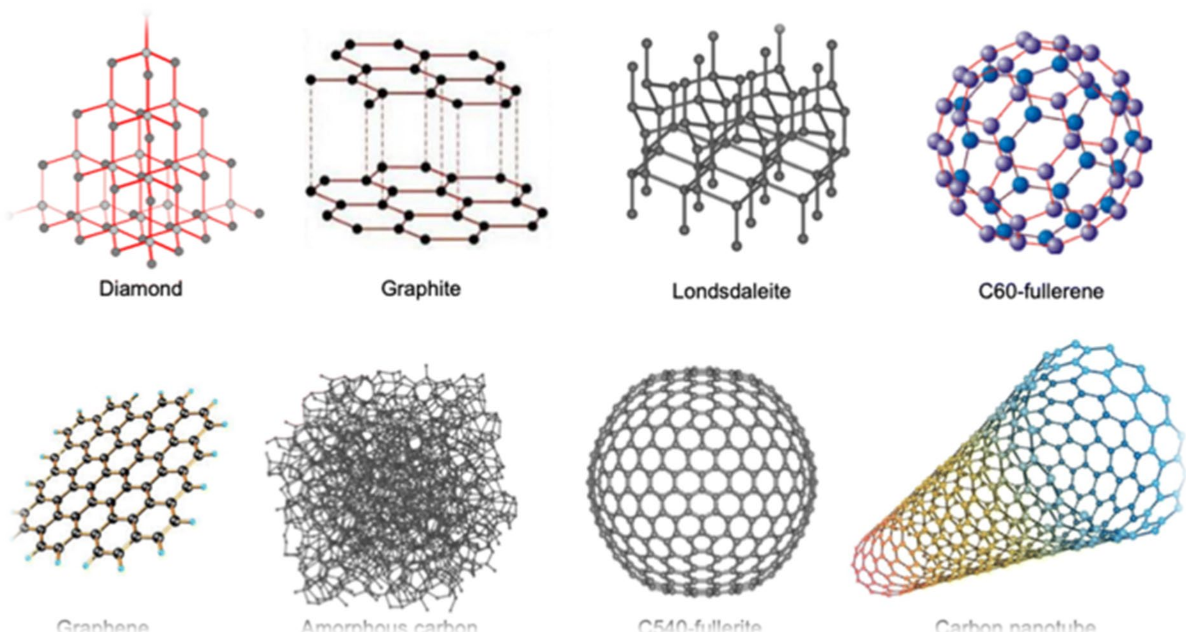


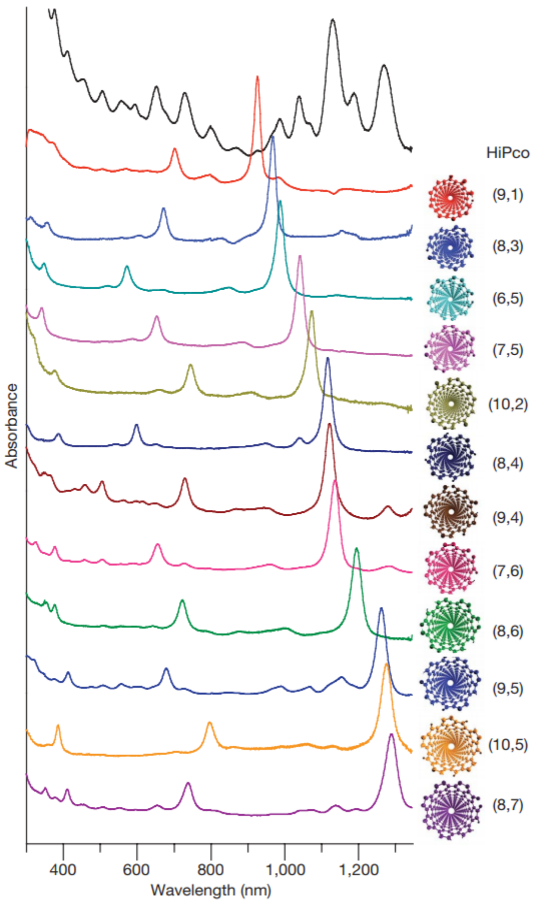
Amit Joshi et al, *Nature Nanotechnology*, 2008, 3, 41– 45
Chia-Ying Chen et al., *Environmental Science & Technology*, 2010, 44, 6674 – 6679
Cao et al., Chemical Engineering Journal, Volume 431, 2022, 134005

Various carbon materials

Carbon nanotubes (CNTs) & photodynamic effects

- Chirality, surface chemistry, electrical conductivity and surface charge, defects, dispersion





Single-Walled carbon nanotubes (SWCNTs)

Ryosuke Fukuda et al., *Carbon*, 2020, 161, 718 – 725
Tu, X. et al., Nature, 460(7252), 250–253.
Numerical simulation of band gaps for CNTs with different chirality. Collaborate with Parameswari Raju.

Generating ROS by photodynamic effects

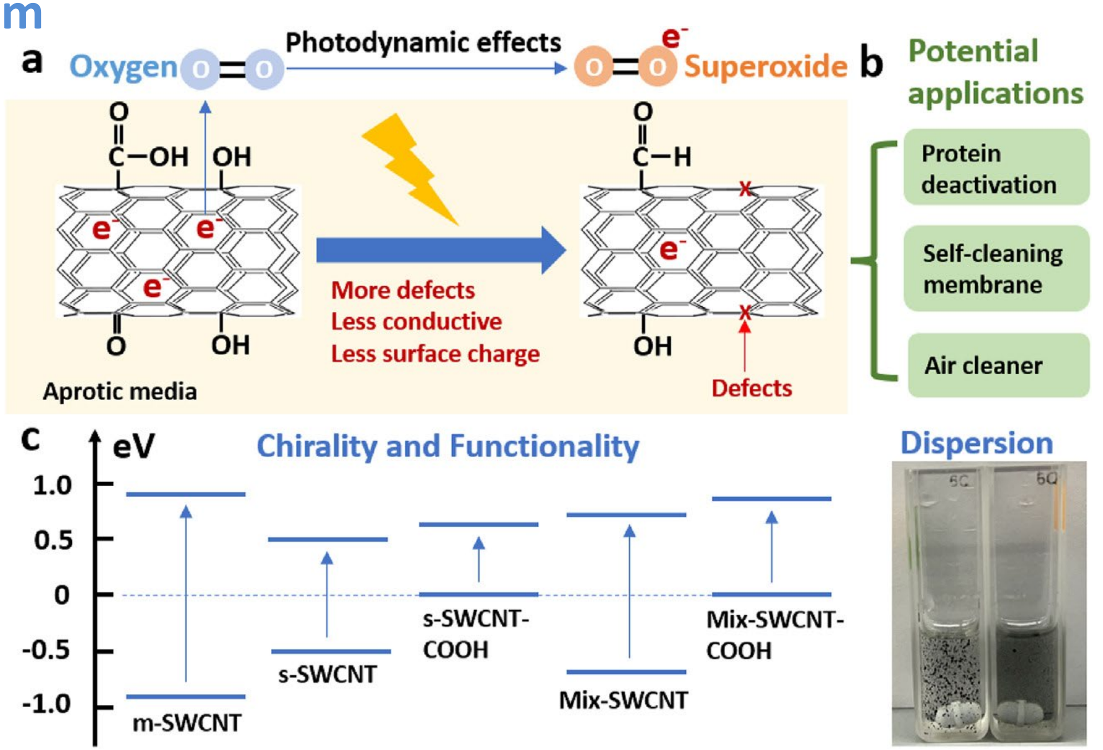
A new system

- Green approach (photon)
- Reusable or last long enough
- Inert environment

Ionic Liquid (IL): [C4mpy][NTf2]

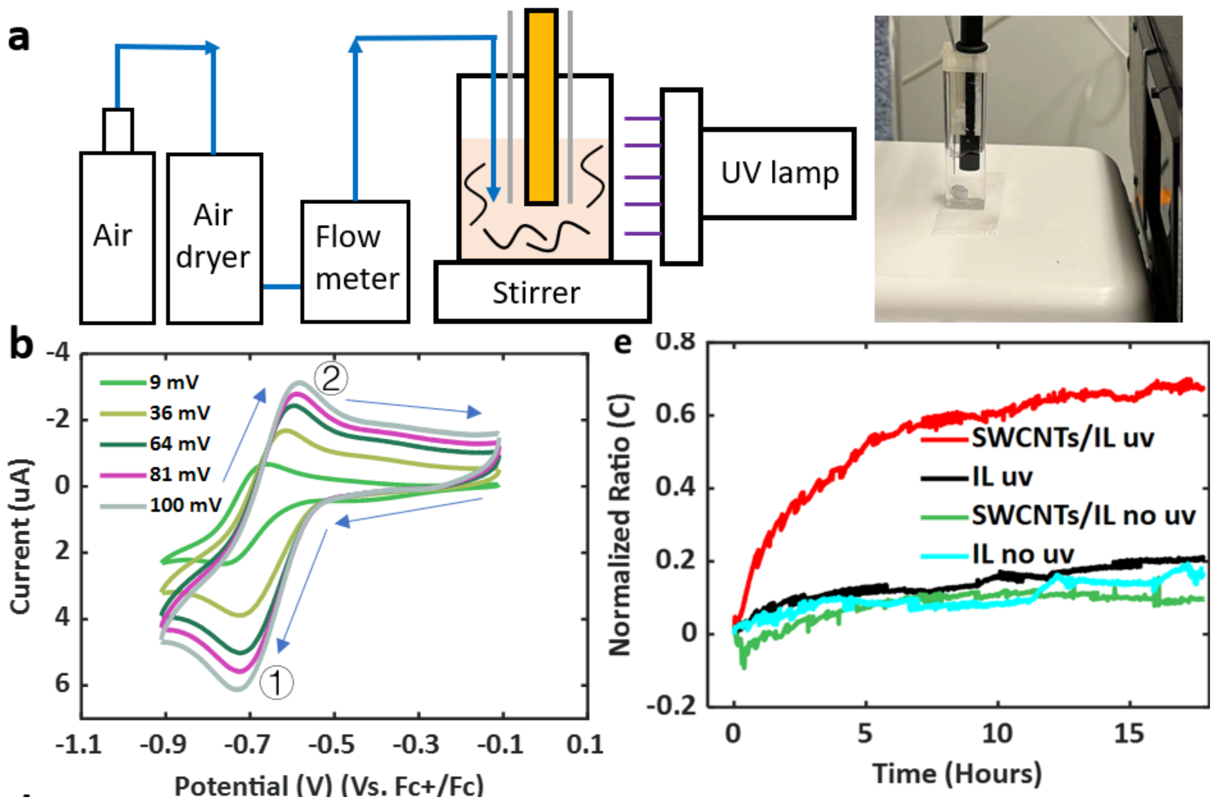
- 1-Butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide
- Store 9 hour*

SWCNT/IL system



*X. Huang, et. al, Materials Today Sustainability, 19, 2022, 100171
X. Huang et. al, Materials Today Energy, 32, 101242, 2023

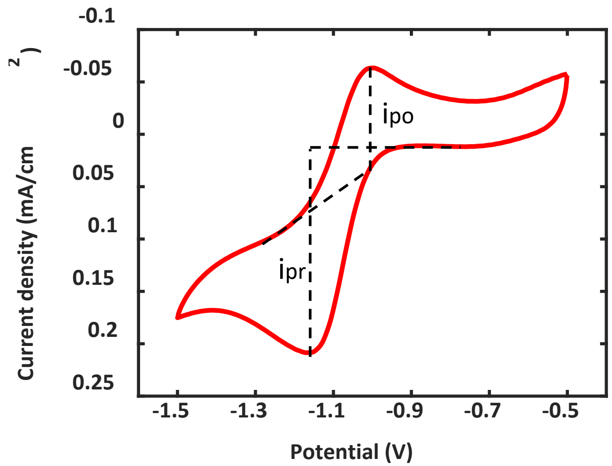
O_2^- calculation & *In-situ* monitor

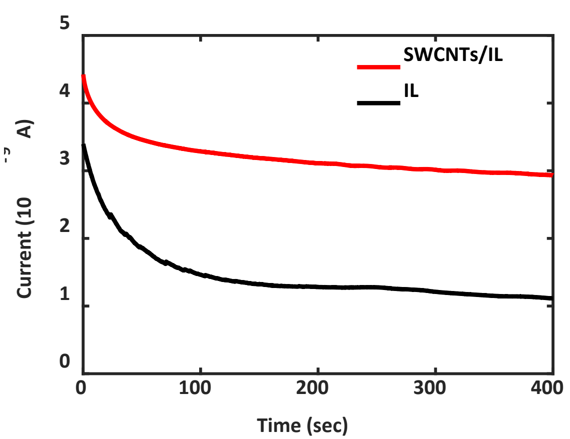


	C_o (mmol)	D_0 (10^{-9} m^2/s)	α	i_{ss} (nA)
Suspension	0.43	2.8	0.36	2.897
IL	1.33	0.33	0.44	1.070

In-situ quantification for O_2^- generation

Cyclic voltammetry and chronoamperometry (CA): oxygen consumption





- ***In-situ* monitoring for O_2^-**

$R(t) = i_{po}(t)/i_{pr}(0)$ $\quad$ $C(t) = [R(t) - R(0)]/R(0)$

- **Equations to calculate O_2^- %**

peak current

$$i_p = (2.99 \times 10^5)\alpha^{0.5} A C_o D_o^{0.5} v^{0.5} \qquad (1)$$

$C_o\, D_o^{1/2}$ --- Eq 1 by CV

$$i_{ss} = 4nFD_oC_or_o \qquad (2)$$

$C_o\, D_o$ --- Eq 2 by CA

$$|E_p - E_{p/2}| = \frac{1.857RT}{\alpha F} \qquad (3)$$

α --- Eq 3 by CV

$R = i_{po} / i_{pr} = C_x D_x / C_o D_o$

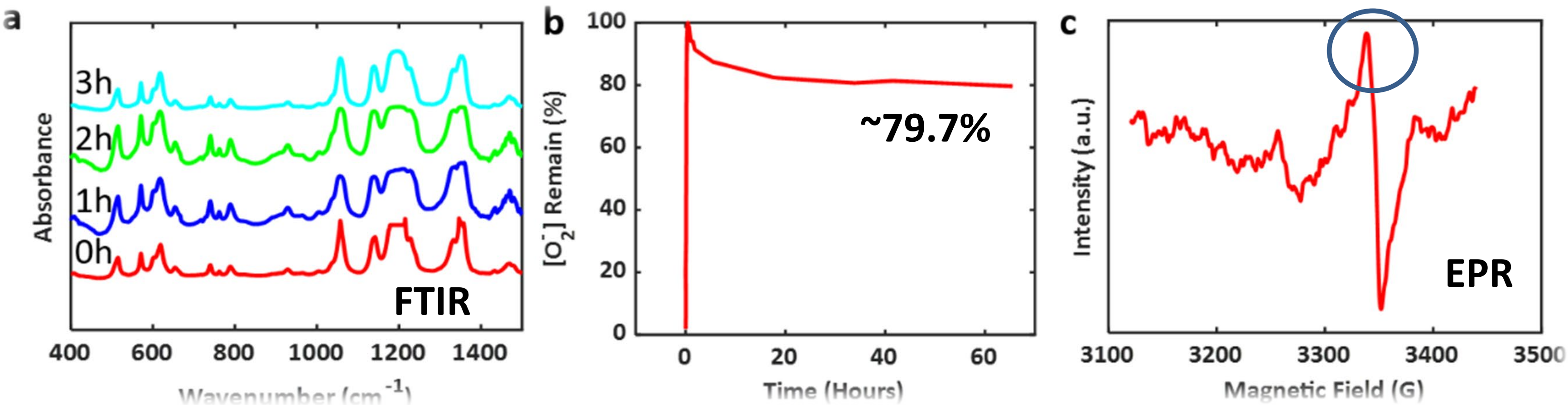
α: charge transfer coefficient; A: the surface area of the working electrode; C_o : the bulk concentration of O_2; D_o: diffusion coefficient of O_2; v: scan rate in V/s; E_p: the peak potential; $E_{p/2}$: the half-peak potential in V; R: the universal gas constant. C_x: $[O_2^-]$; D_x: the diffusion coefficient of O_2^-.

[1] A.J. Bard, L.R. Faulkner, Electrochemical Methods: Fundamentals and Applications, Wiley, New York, 2001.

Sustainable IL system

IL: No change -> Reusable, also supported by UV-vis

Store superoxide for more than 65 hours



Electron paramagnetic resonance (EPR)

SWCNTs

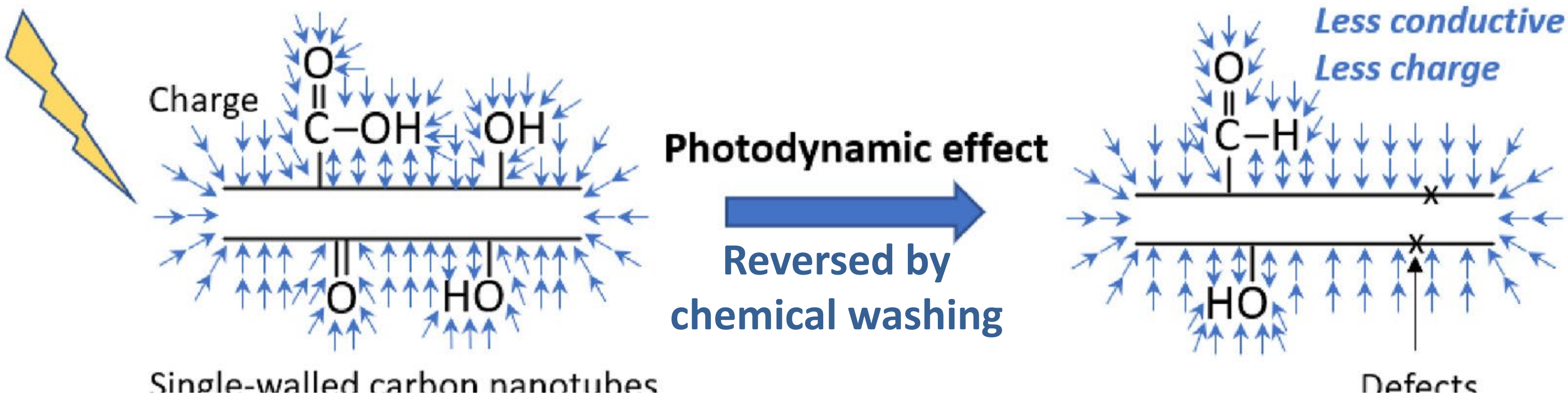
In-situ characterization through Conductive-AFM (C-AFM)

- Resistance increase
- Voltage increase after irradiation

Sustainable system for disinfection

Table 1
Conductive atomic force microscopy and kelvin probe force microscopy results for ultraviolet-treated and non-treated s-single-walled carbon nanotubes .

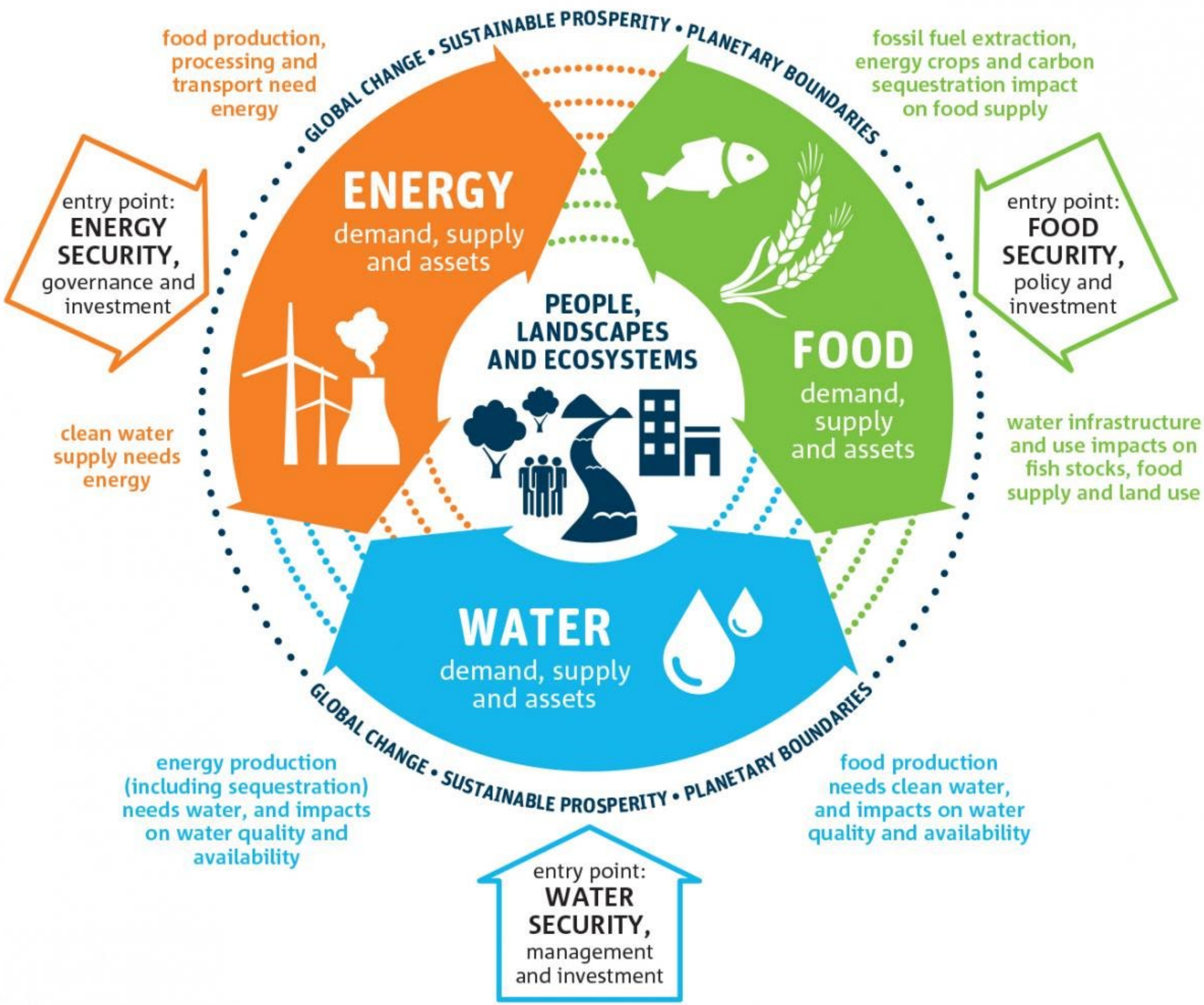
s-SWCNTs	C-AFM	KPFM
	Conductivity (nA)	Potential (mV)
UV-treated	44.08 ± 0.47	−33.15 ± 1.51
Non-treated	50.79 ± 1.00	−66.85 ± 2.66



Ongoing bacteria & virus tests

Changes in s-SWCNTs' surface chemistry, including lower in sp2/sp3, decreased atomic content of p-p*, and reduced surface functional groups.

Other efforts: Water-energy-food nexus



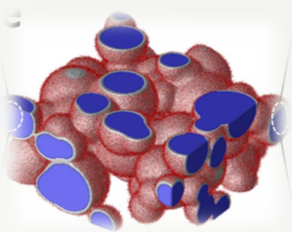
Iman Nuwayhid, et. al, Front. Envion. Sci, 10, 2022, 879081

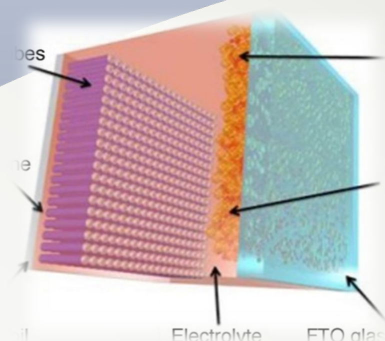
Future work: Smart system by design

Reliable, affordable, and available

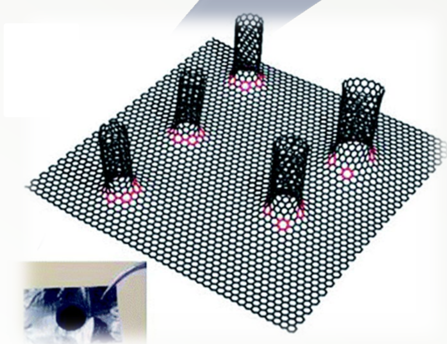
Integrated System

Hybrid & Hierarchical Materials Enabled Device





Materials



Acknowledgement

Group members:

- Dr. Rui He (graduated); Dr. Xiaozhou Huang (graduated); John Shea; Pengxi Zhu; Siyuan Wang, Boshen Xu
- Crystal Bowers, Samuel Athapaththu, Ashley Kong, Ali Boldaji, Chengbo Huang, Akai A Senthill, Mohammad Sheran

Collaborators:

- Prof. Qiliang Li, Prof. Monique Van Hoek

Thank you!

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