NanoCat Group

www.nanocat.co.in

Nanocatalysis to Combat Climate Change

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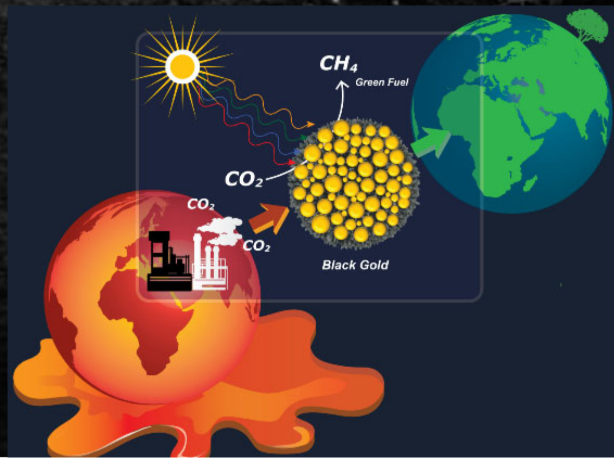
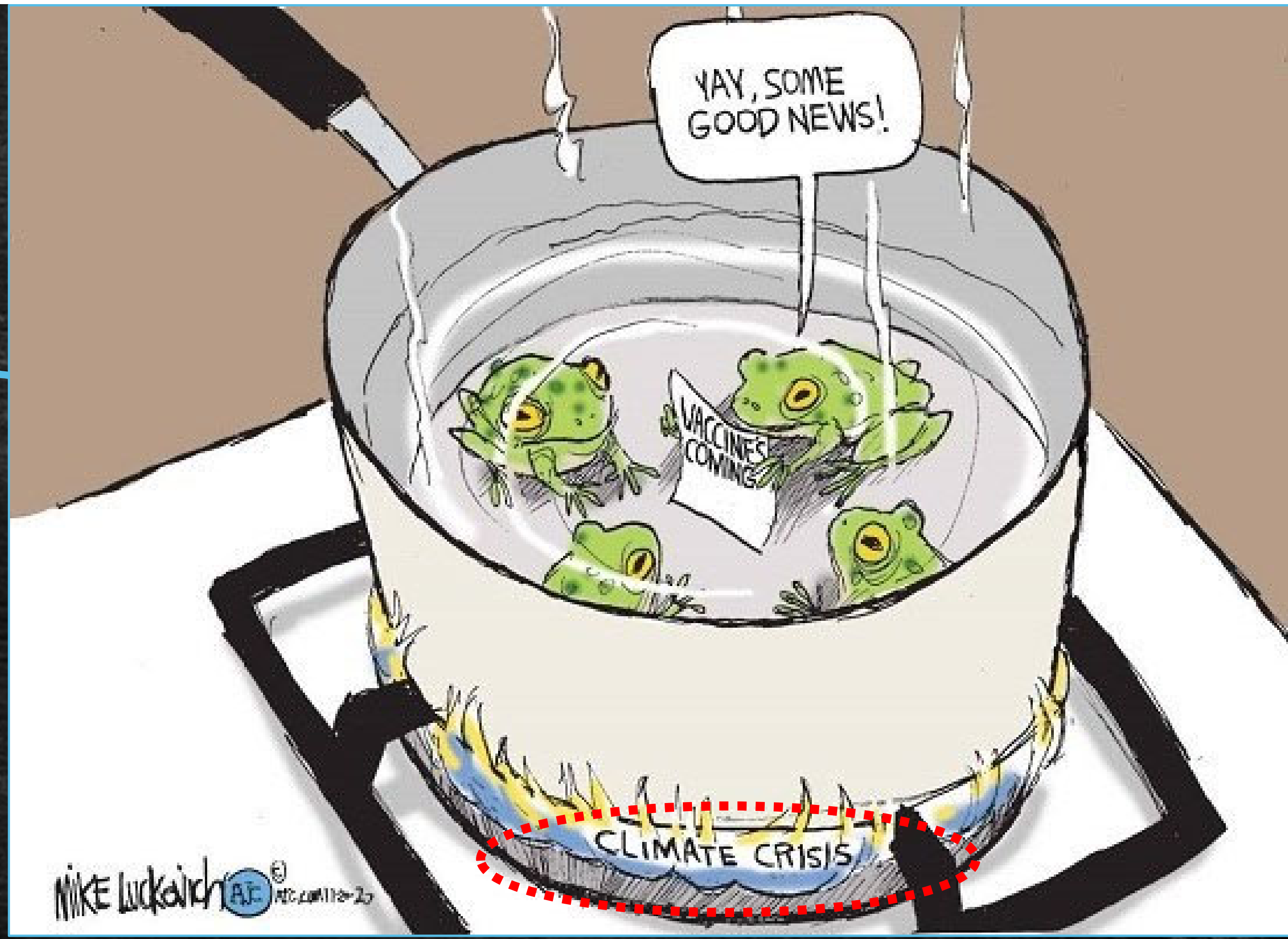
Tata Institute of Fundamental Research
(TIFR), Mumbai



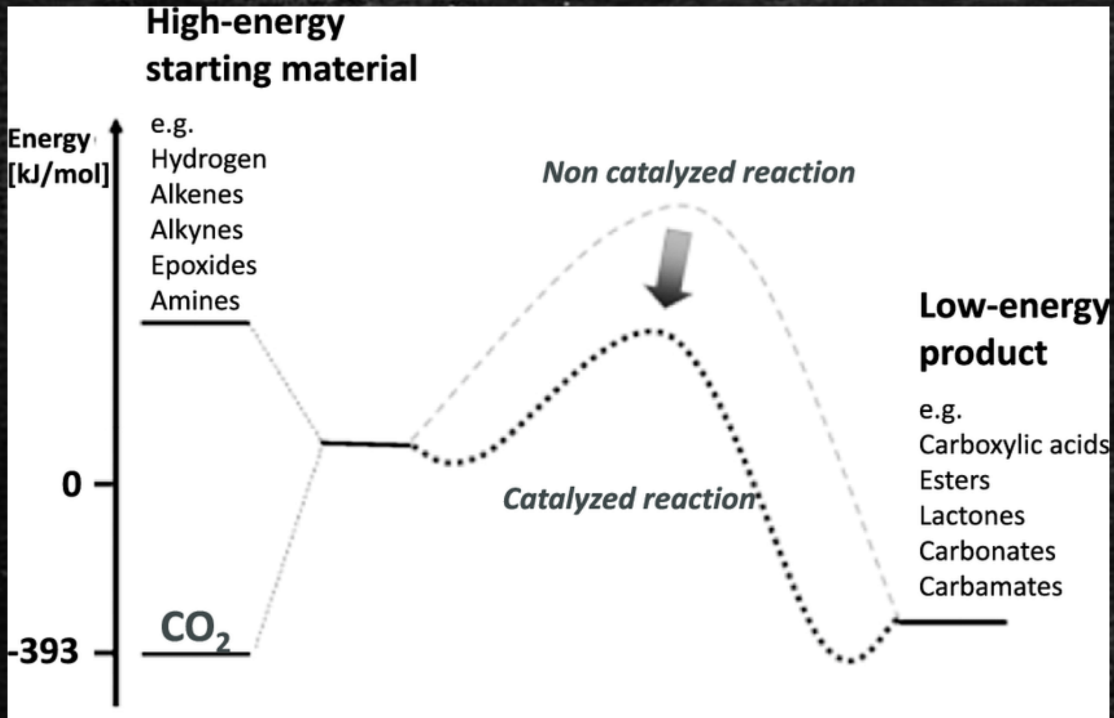
CLIMATE CHANGE due to excessive carbon dioxide (CO_2) is the "Most Serious Problem Mankind Has Ever Faced".



"The capture and utilization of carbon dioxide using solar energy and renewable hydrogen should become the preferred path to manufacture chemicals and fuels"

CO_2 Conversion is the Challenging Process

CATALYSTS & NANOMATERIALS can help reduce activation energy barrier & also harvest solar energy



Alper et al. 10.1016/j.petlm.2016.11.003

"STORING SUN ENERGY IN CO_2"

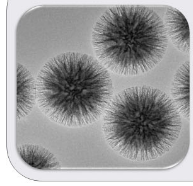
"CO_2 conversion to fuel using renewable H_2 can provide a solution to these two problems of,

i) excessive CO_2 levels, and

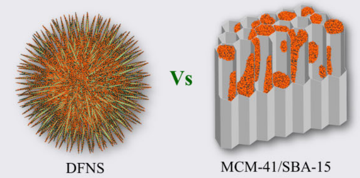
ii) the temporal mismatch between renewable electricity production and demand as well as H_2 storage"

Nanocatalysis Laboratory
(to Combat Climate Change)

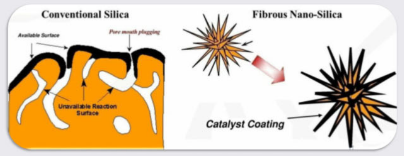
Dendritic Fibrous Silica Nano-Silica (DFNS)



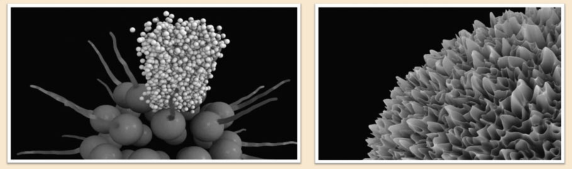
- Nano-Silica (120 to1200 nm)
- High surface area (up to1200 m^2/g)
- High thermal stability (up to 950 °C)
- Hydro-thermal stability
- Excellent mechanical stability
- Fibrous surface morphology



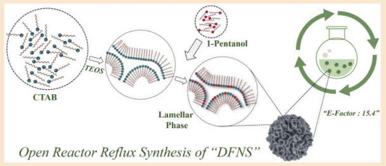
Accessibility of Active Sites



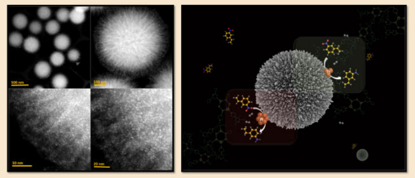
Formation Mechanism, Size and Fiber Density Control of DFNS



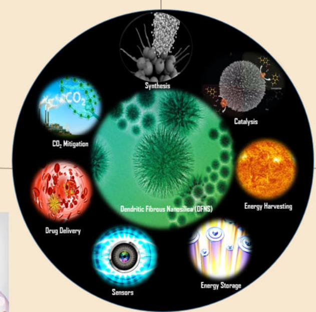
- Dendritic Fibrous NanoSilica (DFNS)
- NanoTitania
- NanoTantalumOxide
- NanoCarbon
- NanoSilicaAluminate

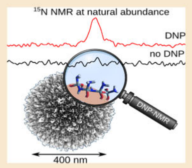


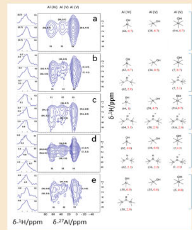
Morphology Controlled Nanocatalysts



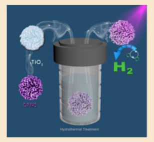
- Insights into the Catalytic Activity of Nitrated Fibrous Silica
- Tuning the Activity of SBA-15-Oxynitrides Solid Bases
- Sustainable Protocols for Supported Metal Nanocatalysts
- Ultrasmall NPs and Pseudo Single Atoms of Pt and Au based Catalysts with High TON and FOM
- Silica-BN for Catalytic Propane to Propene
- Aluminosilcates and Ironsilicates for C-H Activation

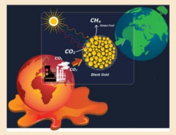


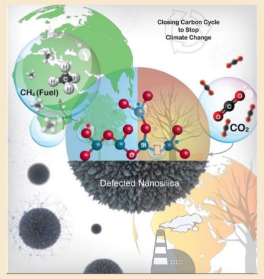




Nanomaterials for CO_2 Capture & Conversion







- Making DFNS Photoactive by Coating of TiO_2 on its Fibers using ALD and Solution Phase Protocols
- Use of DFNS as Hard Template for the Synthesis of High Surface Area Nanostructured Metal Oxides
- Design of Plasmonic Nano-Catalysts for Harvesting Solar Energy
- Hot Spot Engineering by Tuning Interparticle Plasmon Coupling
- CO_2 Methanation using Black Gold
- Defect Catalysed CO_2 Conversion

Selected Publications from our Group

ACS Sus. Chem. Eng. **2013**, *1*, 1192
Angew. Chem. Int. Ed. **2015,** *54*, 2190
Angew. Chem. Int. Ed. **2015,** *54*, 5985
J. Mat. Chem. A, **2016**, *4*, 7005; **2016**, *4*, 12416
ACS Catal. **2016**, *6*, 2770

Green Chem. **2016**, *18*, 5890,
ChemPlusChem **2016**, *81*, 1142
ChemSusChem, **2017,** *10*, 2182 & *10*, 3866
J. Mat. Chem. A, **2017**, *5*, 1935 & *5*, 14914
J. Phy. Chem A. **2017**, *121*, 8080
Langmuir **2017**, *33*, 13774

ACS App. Mat. Int. **2018**, *10*, 23392
ACS App. Nano Mater. **2018**, *1*, 3636
ChemPhotoChem, **2018**, *2*, 796
ChemNanoMat **2018**, 1231
ChemCatChem, **2018**, 881

Nature Prot. **2019,** *11*, 5365
Chemical Sci. **2019**, *10*, 6694
NanoScale, **2019**, *11*, 5365
Proc. Natl. Acad. Sci. **2020**, 6383
Nature Comm. **2020**, *11*, 3828
Langmuir **2020**, *36*, 12755
ACS Materials Lett. **2020**, *2*, 699
ACS Sus. Chem. Eng. **2020**, *8*, 16124
ACS App. Eng. Mater. **2020**, *3*, 8150

Chemical Science, **2021**, *12*, 5774.
Chemical Science, **2021**, *12*, 4825.
Chemical Science, **2021**, *12*, 4267.
Chemical Comm., **2021**, *57*, 2005
Langumir **2021**, *37*, 6423
ACS Materials Lett, **2021**, *3*, 574

Group Members
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Ms. Sushma Kundu
Mr. Rishi Verma
Mr. Rajesh Belgamwar
Mr. Saideep Singh
Ms. Gunjan Sharma
Mr. Pratip Chatterjee

"Guiding Principles"

Catalytic performance (activity, kinetics, selectivity & stability) can be controlled by tuning the active sites (type, size, environment), defects and morphology of nanomaterial support.

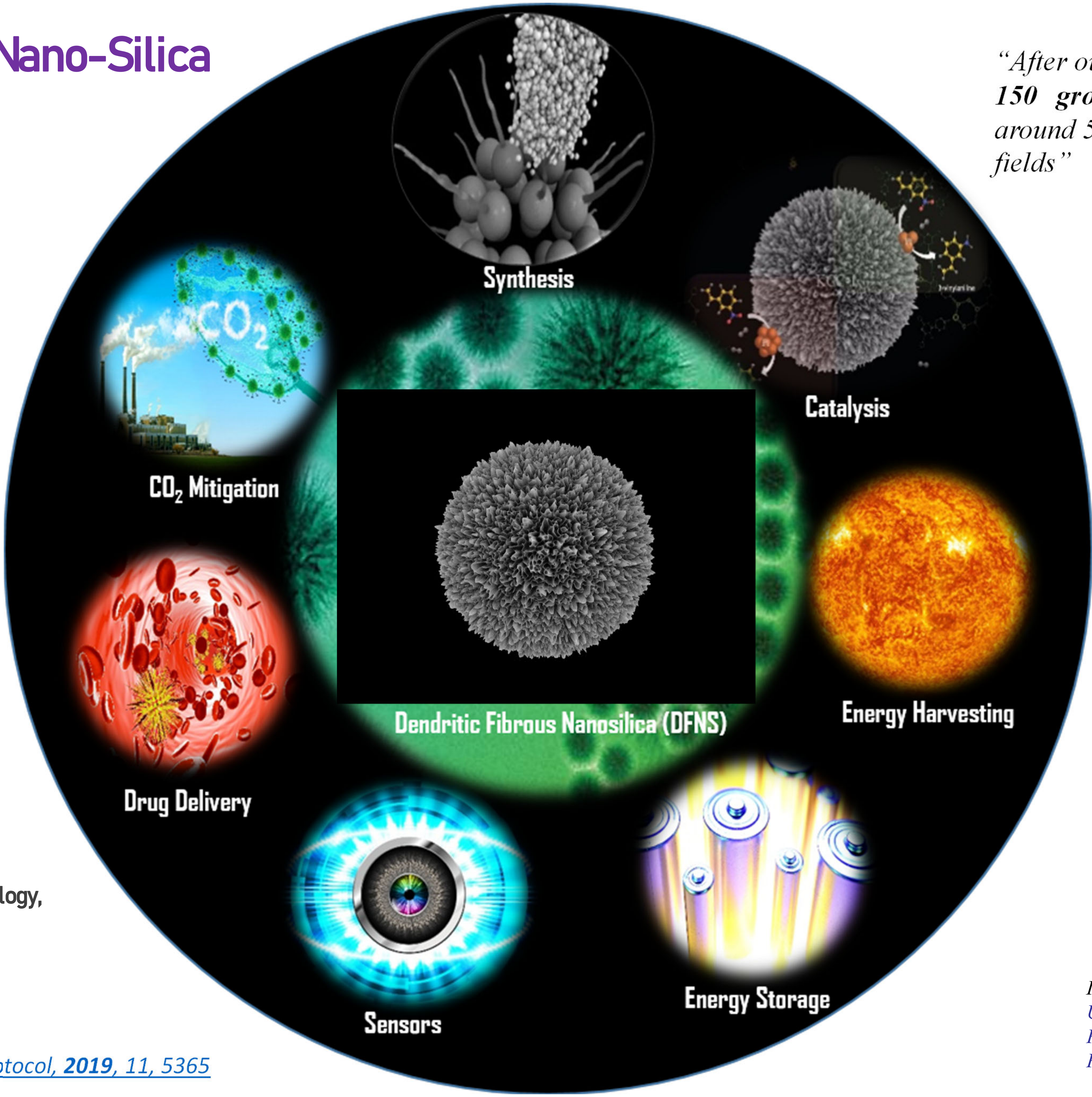
Some of the Breakthroughs from Our NanoCat Lab

Dendritic Fibrous Nano-Silica (DFNS)

"Indian Invented Material used by the World"

- Nano-Silica (50 to 1200 nm),
- High Surface Area (500 to 1200 m^2/g),
- Thermal Stability (up to 800^0C),
- Hydro-Thermal Stability,
- Mechanical Stability (up to 130 MPa),
- Unique Fibrous Surface Morphology,
- Easy to Synthesize.

Maity, Polshettiwar, et al. *Nature Protocol*, **2019**, *11*, 5365



*"After our discovery of DFNS, now more than **150 groups** worldwide using DFNS, with around 500 reports of use of DFNS in various fields"*

Polshettiwar et al.

Angew. Chem. Int. Ed. **2010**, *49*, 9652, *Angew. Chem. Int. Ed.* **2011**, *50*, 2747,

Chemical Science, **2012**, *3*, 2224,

ACS Catalysis **2012**, *2*, 1425;

ACS Sus. Chem. Eng. **2013**, *1*, 1192,

Angew. Chem. Int. Ed. **2015,** *54*, 2190, *Angew. Chem. Int. Ed.* **2015,** *54*, 5985,

J. Mat. Chem. A, **2016**, *4*, 7005; **2016**, *4*, 12416;

ACS Catal. **2016**, *6*, 2770, *Green Chem.* **2016**, *18*, 5890, *ChemPlusChem* **2016**, *81*, 1142,

ChemSusChem, **2017**, *10*, 2182 & *10*, 3866, *J. Mat. Chem. A*, **2017**, *5*, 1935 & *5*, 14914

J. Phy. Chem A. **2017**, *121, 8080; Langmuir* **2017**, *33,* 13774.

ACS App. Mater. Inter. **2018**, *10, 23392; ACS App. Nano Mater.* **2018**, *1, 3636;*

ChemPhotoChem, **2018**, *2, 796; ChemNanoMat* **2018**, *1231; ChemCatChem*, **2018**,*,881.*

Nature Protocol **2019,** *11*, 5365,

Chemical Science **2019**, *10*, 6694;

NanoScale **2019**, *11*, 5365;

Proc. Natl. Acad. Sci. U.S.A (PNAS) **2020**, 6383;

Nature Comm. **2020**, *11*, 3828.

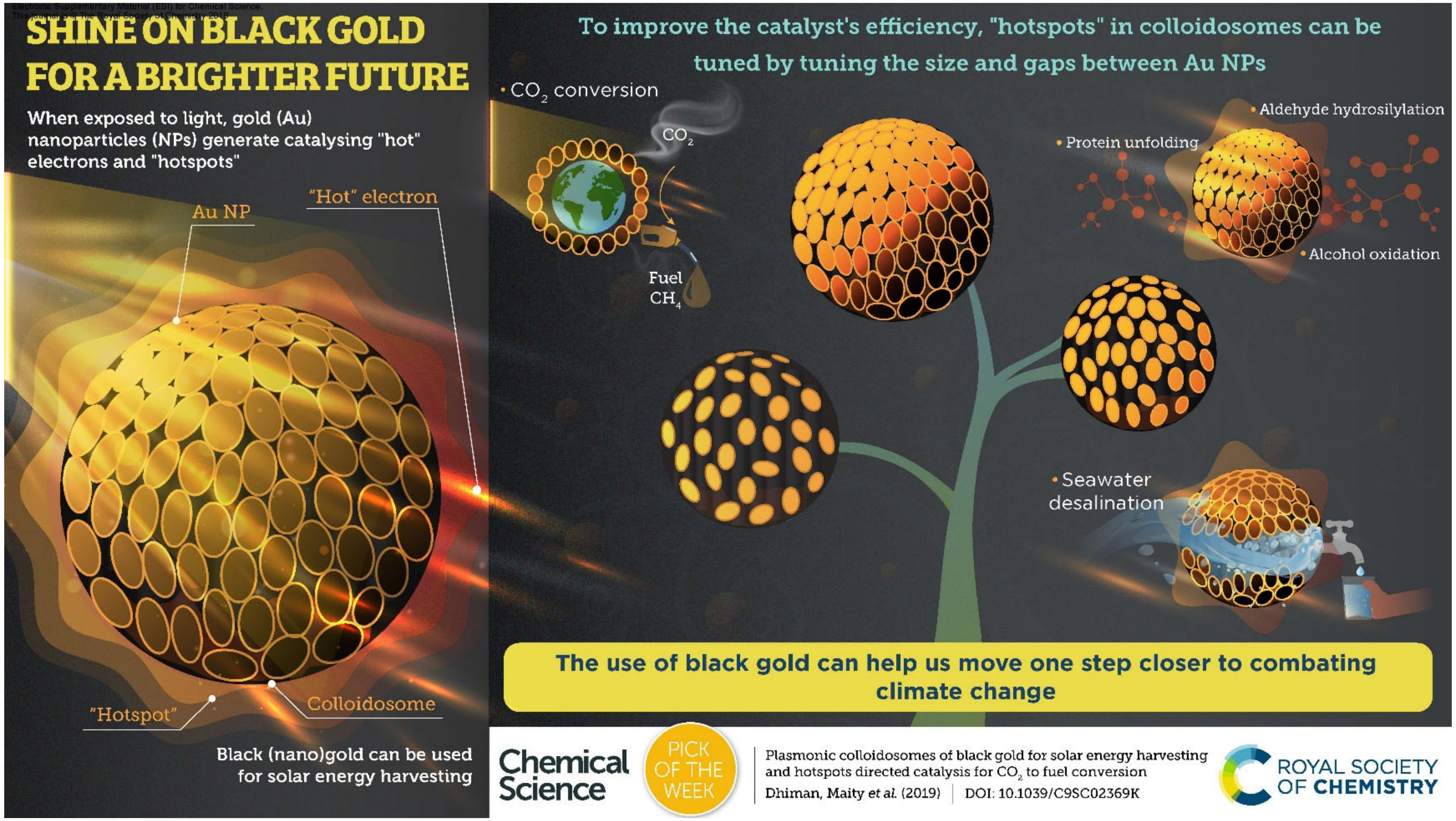
Chemical Science **2021**, *12*, 4285;

Chemical Science **2021**, *12*, 4267;

Chemical Science **2021**, 5774.

International Patents
US Patent US20110253643
PCT/IB2016/051870
PCT/IN2020/050458

Indian Patents
2016-21004089
2020-21001441
2020-21001440
2020-21008717
2020-21040554



Black Gold
: an Artificial Tree

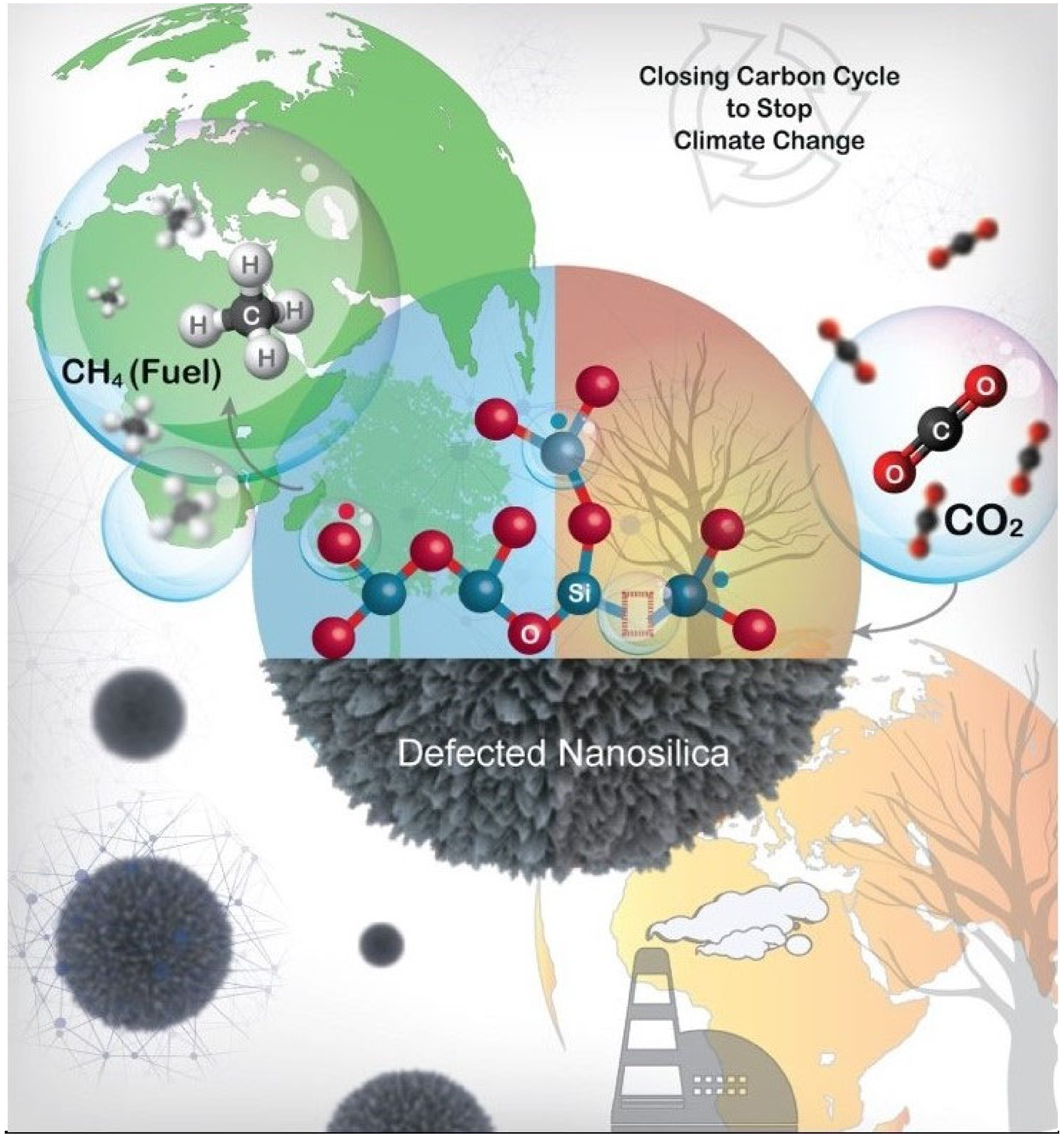
Black Gold absorbs the entire visible and near-infrared region of solar light, due to interparticle plasmonic coupling.

Mr. Mahak Dhiman

Black Gold acts like an artificial tree that uses CO_2, sunlight and water to produce fuel.

It also converts sea water to potable water.

Polshettiwar et al. Chemical Sci. ***2019****, 10, 6694*

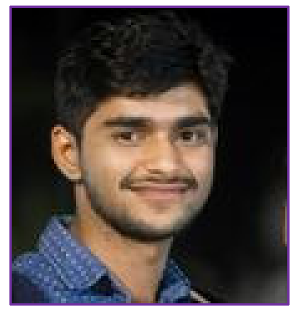


"Perfecting Imperfection"

for CO_2 Conversion

Defects in Nanosilica Catalytically Convert CO_2 to Methane

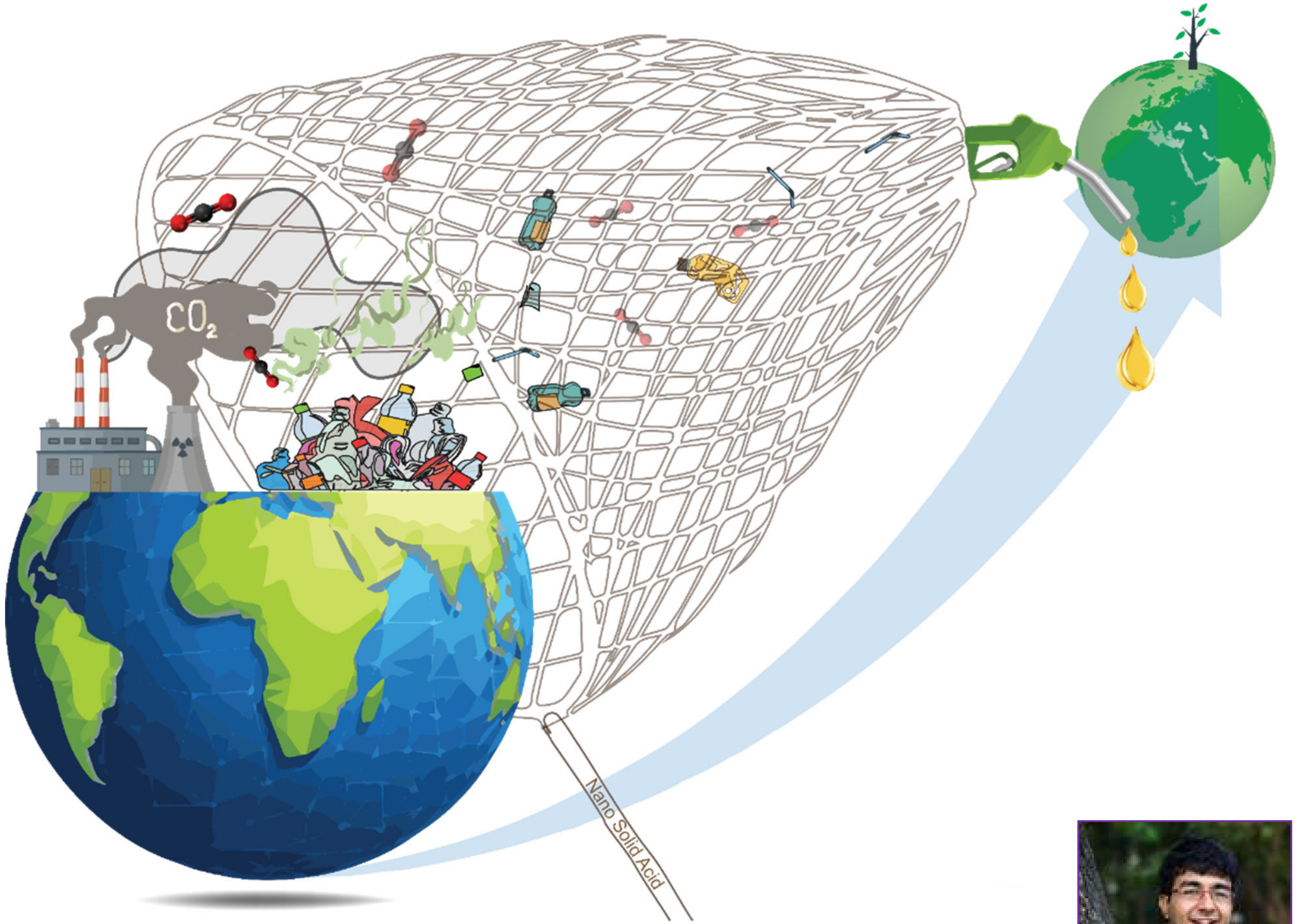
First example of Metal-Free-Ligand-Free CO2 Conversion Process



Mr. Amit Mishra

Polshettiwar et al. Proc. Natl. Acad. Sci. U.S.A (PNAS) ***2020****, 117, 6383.*

“Solid Acids for Waste Plastic and CO_2 Chemicals”



Catalytic Nanosponges of Acidic Aluminosilicates for Plastic Degradation and CO_2 to Fuel Conversion.

Alkanes C5-C21 chain length (53%)

C2-C4 alkenes (46.6%)

Coke (0.4%)

Mr. Ayan Maity

Maity, Polshettiwar et al. Nature Communication ***2020****, 11, 3828.*

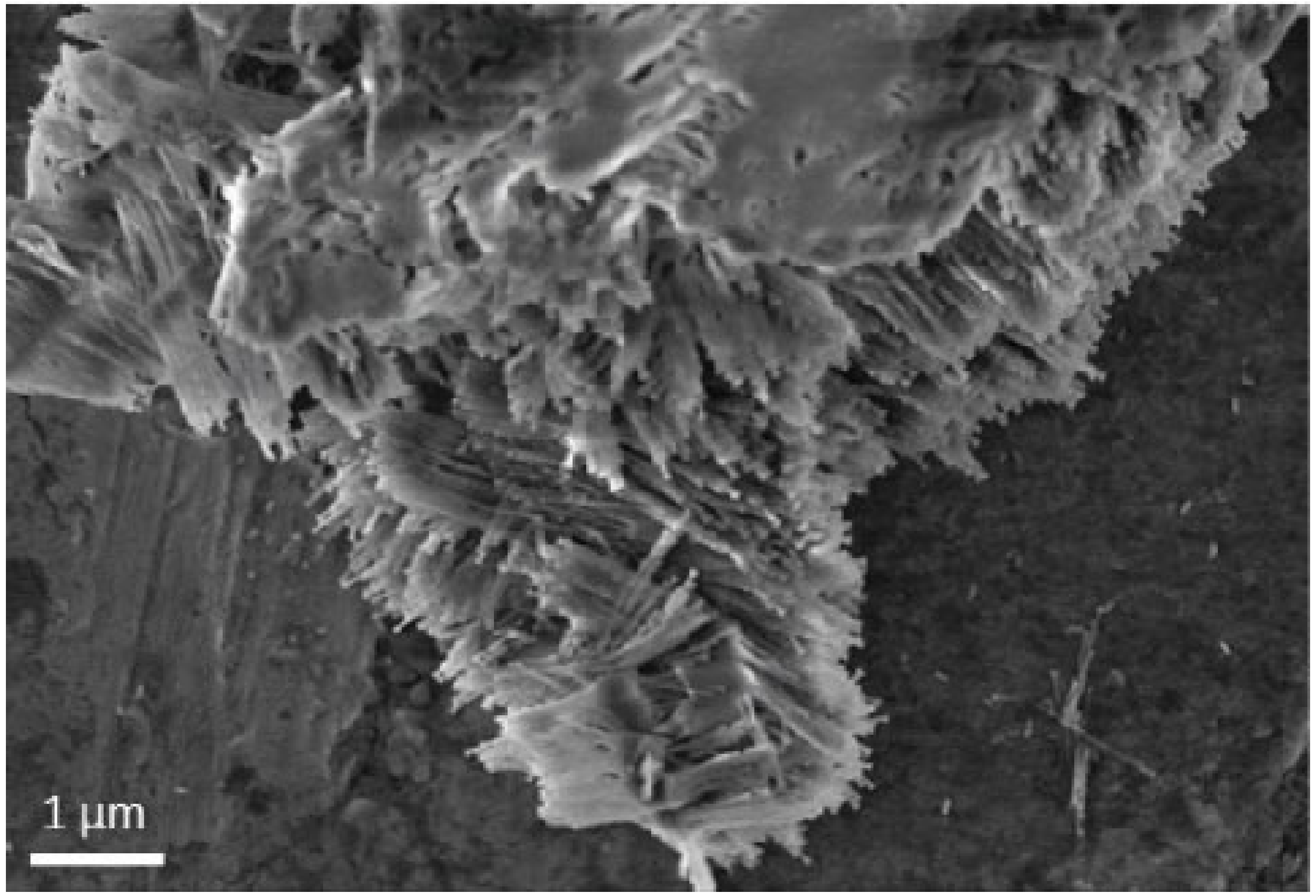
"DNFS based Sorbents for CO_2 Capture"

Capture Good Amount of CO_2 at Moderate Temperature and Atmospheric Pressure. Faster Kinetics, Stable and Recyclable and Selective.

Polshettiwar,* et al. *Chem. Sci.*, **2012**, *3*, 4222; *J. Mat. Chem. A*, **2016**, 4, 7005.

"High Temperature CO_2 Capture"

Lithium silicate nanosheets (LSNs) showed high CO_2 capture capacity with ultra-fast kinetics and enhanced stability, at least 200 cycles.



Belgamwar, Polshettiwar* et al. *Chemical Science*, **2021**, *12*, 4825.

CO_2 Conversion – "Dream Process"

- at ambient temperature and pressure
- without external energy
- water as a hydrogen source
- using an inexpensive and abundant material

Transforming CO_2 and Sea Water to Green HYDROGEN & Green CEMENT Using Magnesium Scrap

"CO_2 to Fuel and Cement at Room Temperature"

Bubble the Air in Water with a pinch of Magnesium and you will get Fuel and Green Cement, at room temperature and pressure.

Polshettiwar et al. Chemical Science, **2021,** *12*, 5774. Patent (PCT) filed 2020.

"Process for CO_2 Conversion"

$$CO_2 + H_2O \xrightarrow[\text{0 to 25 °C}]{\text{MAGNESIUM}} CH_4 + CH_3OH + HCOOH + H_2$$

(or air)

+ Mg-Basic Carbonate

A direct conversion of CO_2 to fuel,

- at room temperature and atmospheric pressure,
- without the need for any external energy (*no light, no electricity, no heat*),
- just using water (*no external hydrogen, even sea water works*).

Magnesium is the 4th most common element in the Earth (after iron, oxygen and silicon), making up 13% of the earth's mass.

"CO_2 will be durably sequestered for more than 100 year in the form of Green Cement"

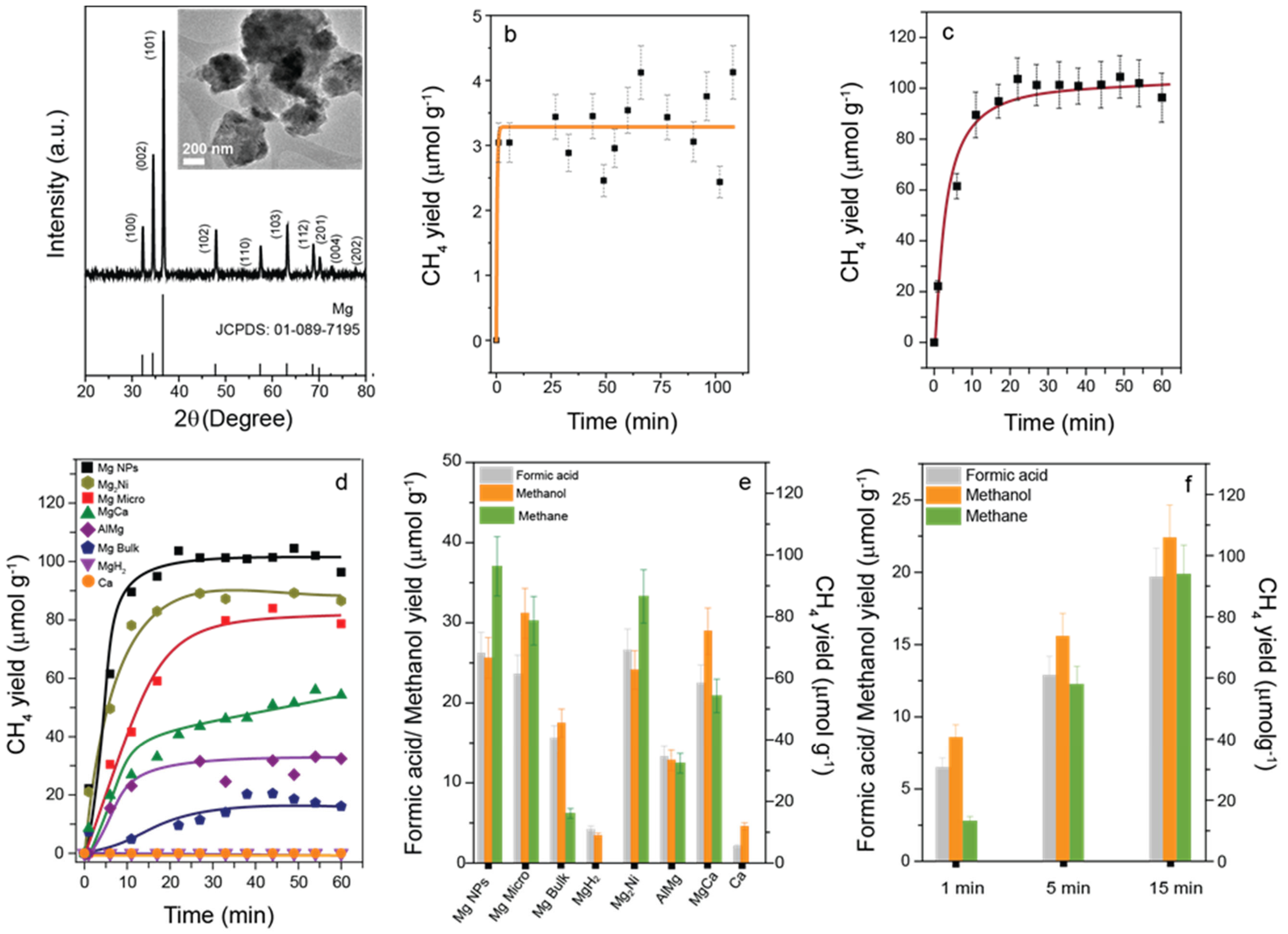
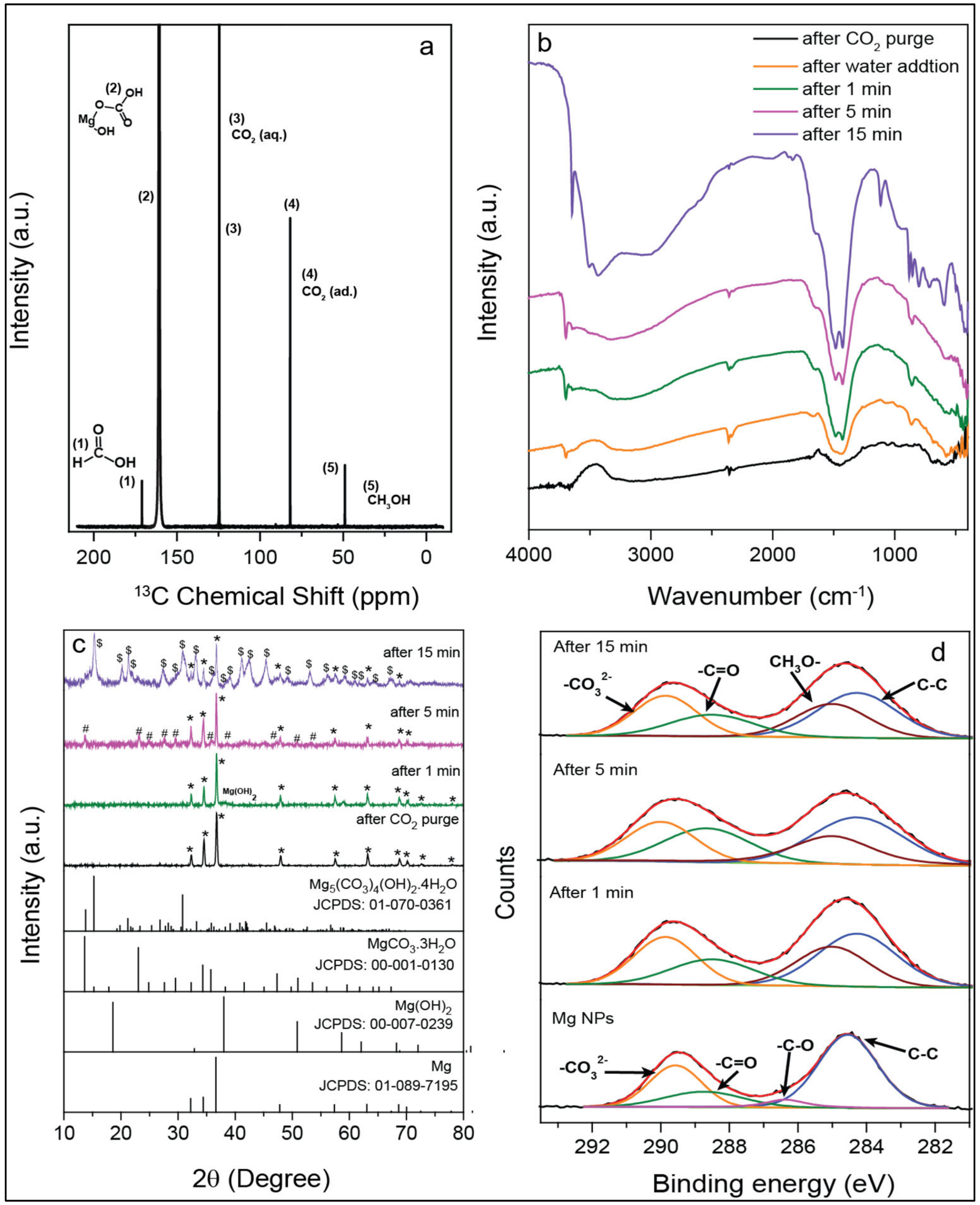


Figure 1. (a) PXRD pattern (TEM image as inset) of Mg NPs along with standard XRD pattern of Mg;

Methane yield with reaction time for CO_2 reduction by Mg NPs using (b) CO_2 directly from the air and (c) 99.99% CO_2

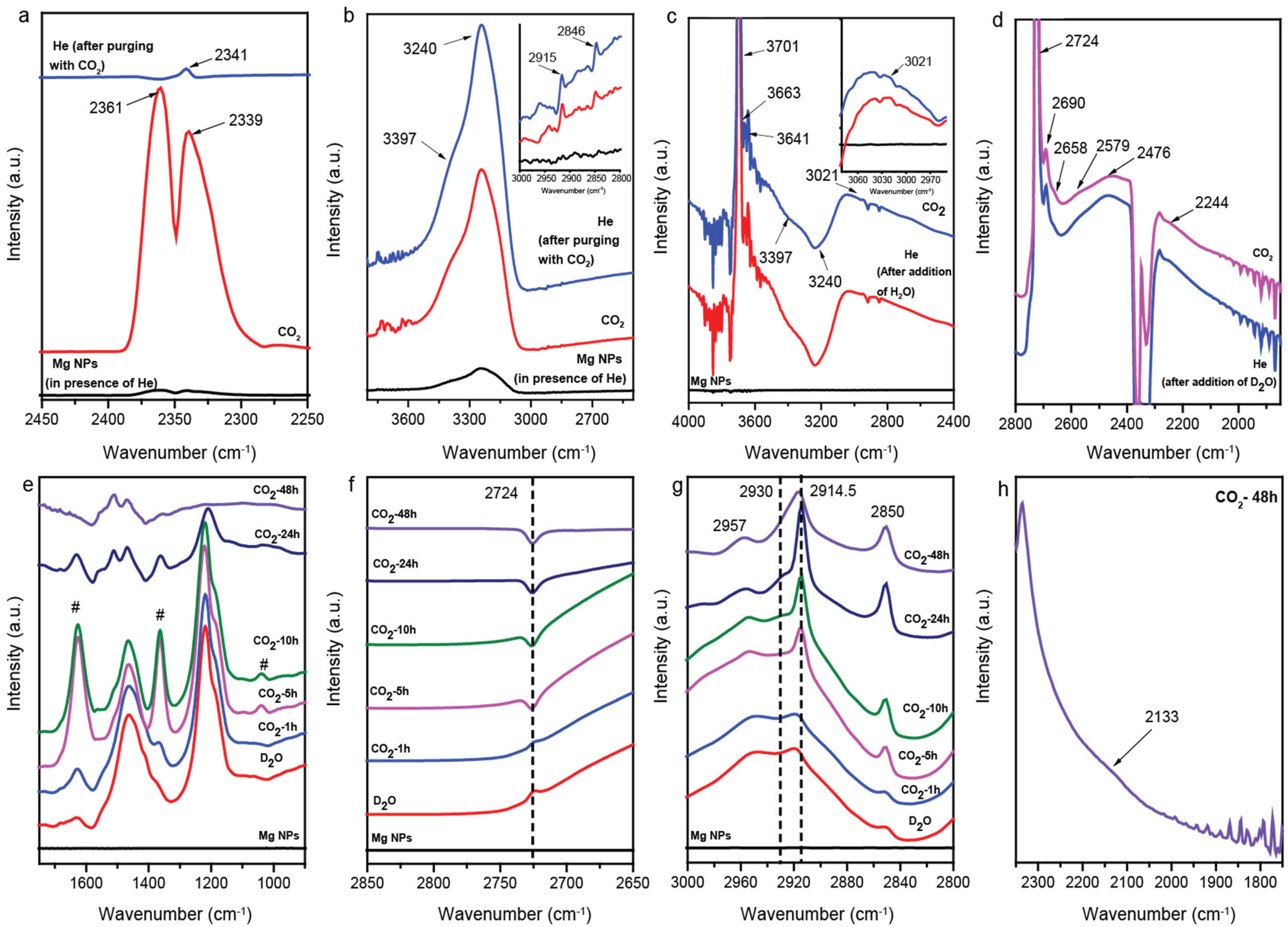


(a) ^{13}**C NMR** spectrum of the reaction mixture (using labeled $^{13}CO_2$) after 1 h of reaction on Mg NPs;

(b) **FTIR** spectra,

(c) **PXRD** patterns and

(d) **XPS** C 1s spectra of solid products recovered after 1, 5, and 15 min of the reaction of CO_2 with Mg NPs and water, at room temperature and atmospheric pressure.



In situ **ATR-FTIR** spectra:

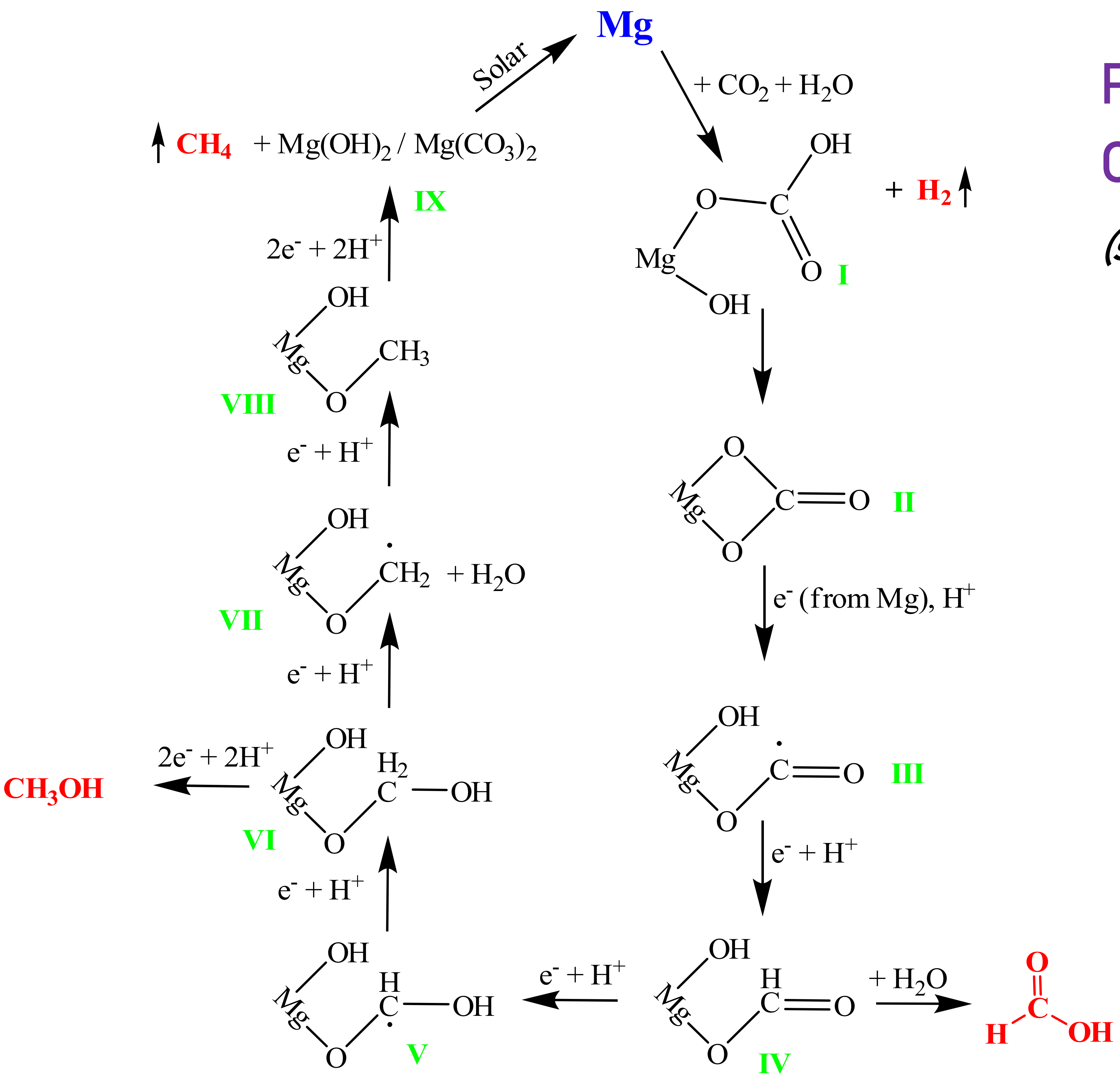
(a) and (b) in He, CO_2, and again He,

(c) after adding H_2O to the Mg NPs and subsequently purging with He and CO_2 gas,

d) after adding D_2O to the Mg NPs and subsequently purging with He and CO_2 gas,

(e-h) after adding D_2O to the Mg NPs and then purging with CO_2 for 1, 5, 10, 24 and 48 h.

Attenuated Total Reflection (ATR)



Plausible reaction mechanism of CO_2 conversion by Mg using water

(supported by in-situ ATR and DFT)

“Process Sustainability”

$$CO_2 + H_2O \xrightarrow[\text{Room Temperature}]{Mg} CH_4 + CH_3OH + HCOOH + H_2 + \text{Mg-Basic Carbonate}$$

1 kg of Mg via simple reaction with water and CO_2 produces in 1 hr,

- Methane (2.43 lit),
- Hydrogen (940 lit),
- Mg-basic carbonate (3.85 kg),
- Small amount of methanol, and formic acid

Mg Basic Carbonate

Mg-Basic Carbonate Uses:
- **Green Cement**
- Ancient building material
- Pharmaceuticals (e.g. antacid and laxatives)
- Flame retardant
- Colour & paints Industries (Fillers for paints, textiles, plastics, etc)

Polshettiwar et al. Chemical Science, ***2021,*** *12,* 5774. Patent (PCT) filed 2020.

"Cost per Tonne"

$$CO_2 + H_2O \xrightarrow[\text{Room Temperature}]{Mg} CH_4 + CH_3OH + HCOOH + H_2 + \text{Mg-Basic Carbonate}$$

1 kg of Mg via simple reaction with water and CO_2 produces in 1 hr,

- Methane (2.43 lit),
- Hydrogen (940 lit),
- Mg-basic carbonate (3.85 kg),
- Small amount of methanol, formic acid

Price Calculations	Input Cost	Product Cost
1 kg Mg (SCRAP)	USD 2	-
3.85 kg Mg-Basic Carbonate (Current Cost is USD 26)	-	USD 100 (USD 26 x 3.85)
2.43 lit Methane	-	Green
940 lit Hydrogen	-	Green
Total Profit Per Kg Per ton		 USD 98 USD 98000
2.2 kg CO_2 mitigated per kg of Magnesium		

Polshettiwar et al. Chemical Science, ***2021,*** *12, 5774.* Patent (PCT) filed 2020.

Magnesium carbonate basic, SKU 13118-1KG
https://www.sigmaaldrich.com/IN/en/product/sial/13118?gclid=CjwKCAjwopWSBhB6EiwAjxmqDRbJc1mD9FSzorF03NM2tCzf8KW4UeAkKCpIaiDGpA6PVfsi5Il9thoC7AsQAvD_BwE

“Life-Cycle Assessment (LCA)” Preliminary (not comprehensive)

Process	Energy (+ required or - produced)		CO_2 (+ released or - mitigated)
Electrolysis of Mg^{2+} to produce 1 Kg Mg	+ 0 MJ Use of Magnesium SCRAP		+ 0 kg Use of Magnesium SCRAP
CO_2 conversion by 1 kg Mg	No external energy was required for this reaction	0 MJ	
	Product-Methane: Energy (50.1 kJ/g) released by burning 1.6 g of Methane	-0.0816 MJ	0.0044 kg (mitigated) 0.1 mol CO_2 converted to methane - 0.1 x 44 = 4.4 g
	Product-Methanol: Energy (22.7 kJ/g) released by burning 0.8138 g of Methanol	-0.0185 MJ	0.0011176 kg (mitigated) 0.0254 mol CO_2 converted to methanol -0.0254 x 44 = 1.1176 g
	Product-Formic Acid: Energy (6.4 MJ/lit) released by burning 0.98 mL of Formic Acid	-0.00627 MJ	0.001196kg (mitigated) 0.026 mol CO_2 converted to formic acid-0.026 x 46 = 1.196 g
	Product-Hydrogen: Energy (0.490 MJ/kg) required to produce 0.083kg hydrogen from fossil fuel (steam reforming of methane), which is saved by this process	-0.0406 MJ	- 0.76 kg (stopped from releasing to the environment) 9.21 kg CO_2 per kg H_2 emitted if produced from methane reforming, i.e. 0.76 kg CO_2 could have been emitted if H_2 was produced from methane.
	Energy (141.86 MJ/kg) released by burning 0.083 kg hydrogen	-11.77 MJ	0 kg (no emission)
	Product- Mg Basic Carbonate: Mg basic carbonate (heat of formation of carbonate)	-2.08 MJ	- 1.44 kg (mitigated) 1 kg Mg produced 3.85 kg basic carbonate by reacting with 1.44 kg CO_2
	Total	**11.91 MJ (Energy generated)**	**2.2 kg (CO_2 mitigated)**

Magnesium (Mg) SCRAP, Energy and Scalability

Amount of Magnesium SCRAP needed

For capturing and converting 1000 tonnes of CO_2 per year (into 3850 tonnes of GREEN CEMENT),
We need 690.79 tonnes of Mg SCRAP per year

Availability of Magnesium SCRAP

In 2016 total magnesium consumption worldwide was 843kt, with production at 878kt. (just 0.08 % scrap per year)

International Magnesium Association

http://www.themtalcasting.com/magnesium-scrap.html

Energy and Water

- without the need for any external energy (*no light, no electricity, no heat*),
- just using water (*even sea water works*).

Scalability

Current scale: 1 gm

Simple mixing of Mg powder, water and CO_2 (air) at room temperature and atmospheric pressure

Waste to Wealth

"CO_2 will be durably sequestered for more than 100 year in the form of Green Cement using scrap (waste) Magnesium"

“Process Sustainability”

$$CO_2 + H_2O \xrightarrow[\text{Room Temperature}]{\text{Mg}} CH_4 + CH_3OH + HCOOH + H_2 + \text{Mg-Basic Carbonate}$$

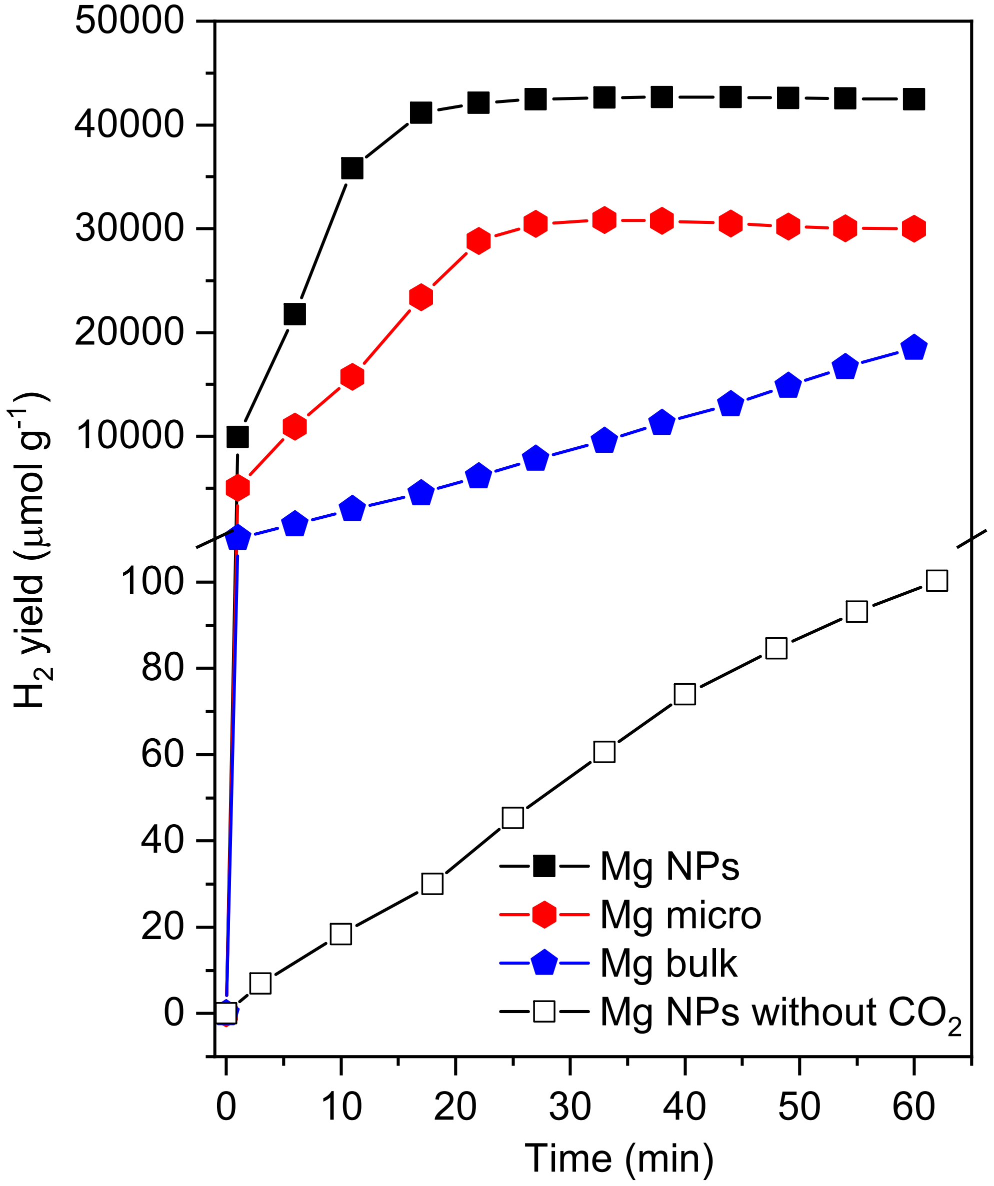
1 kg of Mg via simple reaction with water and CO_2 produces in 1 hr,

- Methane (2.43 lit),
- Hydrogen (940 lit),
- Mg-basic carbonate (3.85 kg),
- Small amount of methanol, and formic acid

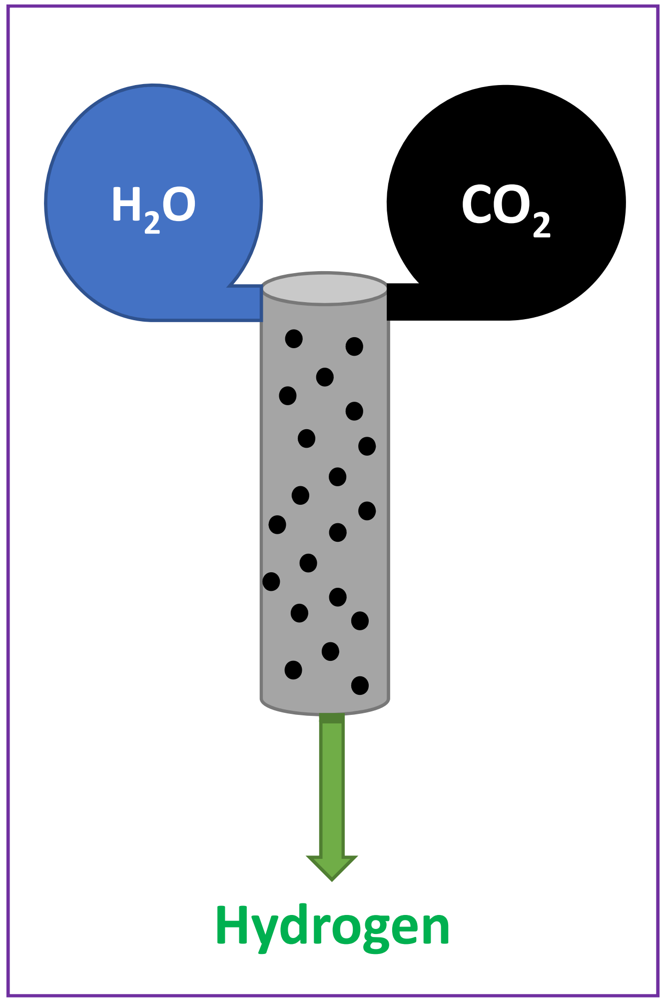
Green Hydrogen

Polshettiwar et al. Chemical Science, **2021,** *12,* 5774. Patent (PCT) filed 2020.

Our Mg protocol can even be used for H_2 production (940 liter per kg of Mg), which is nearly 420 times more than H_2 produced by the reaction of Mg with water alone (2.24 liter per kg of Mg).



"Green Hydrogen on Demand"

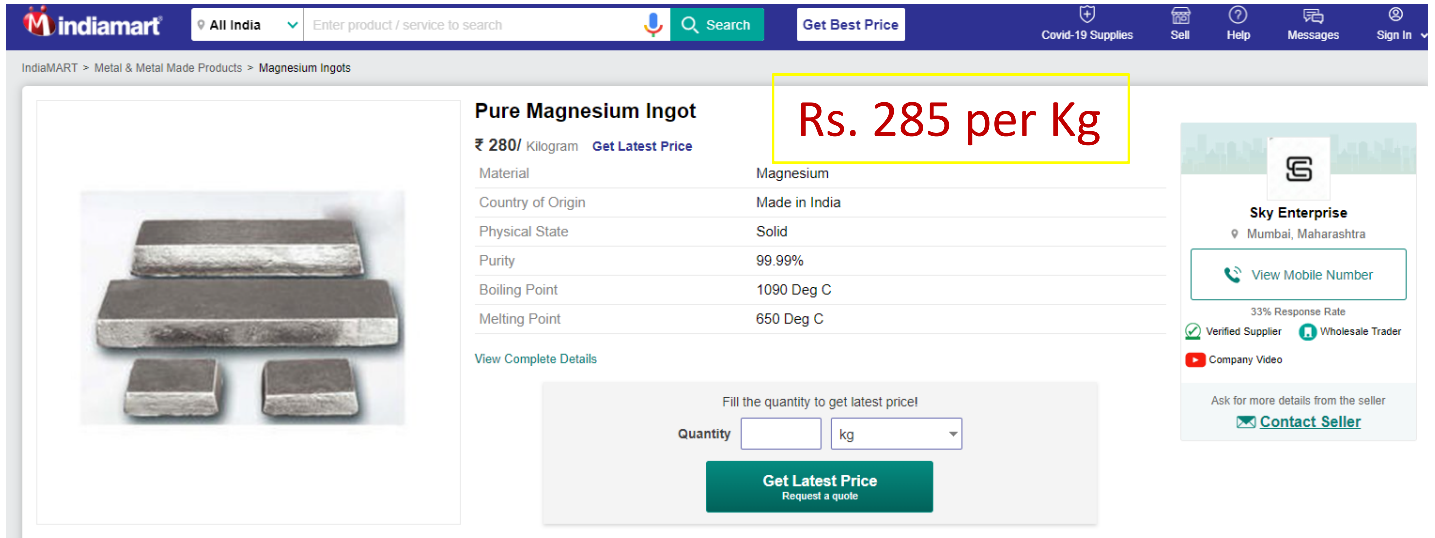


Portable Magnesium Cartridge which will produce
H_2 from Water and CO_2
at Room Temperature and Atmospheric Pressure

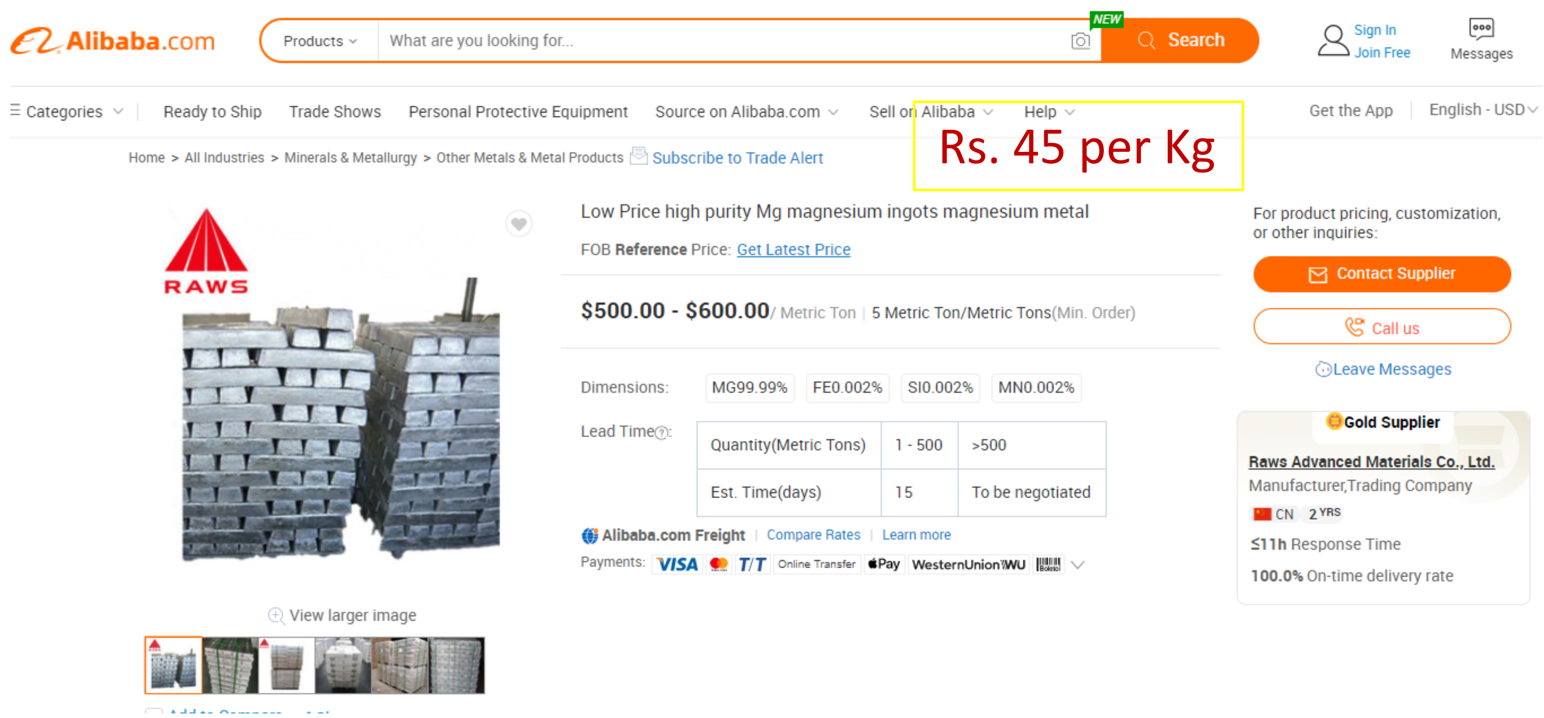
Green Hydrogen

Price of Mg Metal

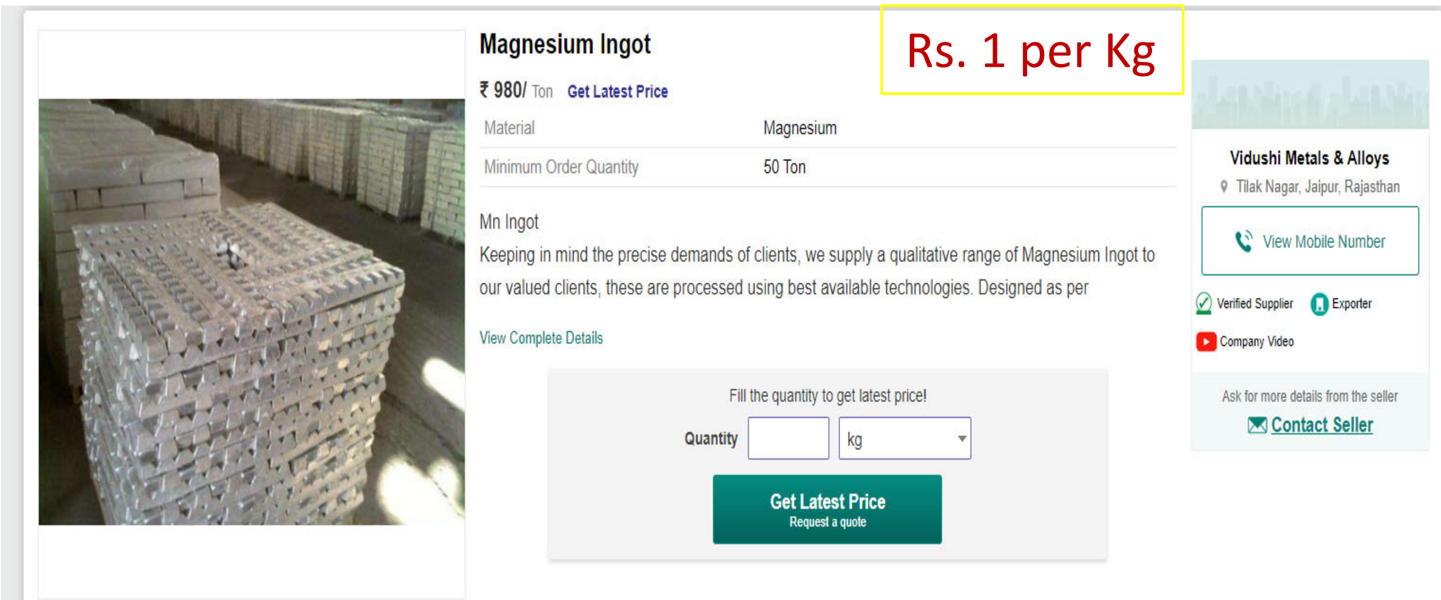
Rs. 285 per Kg



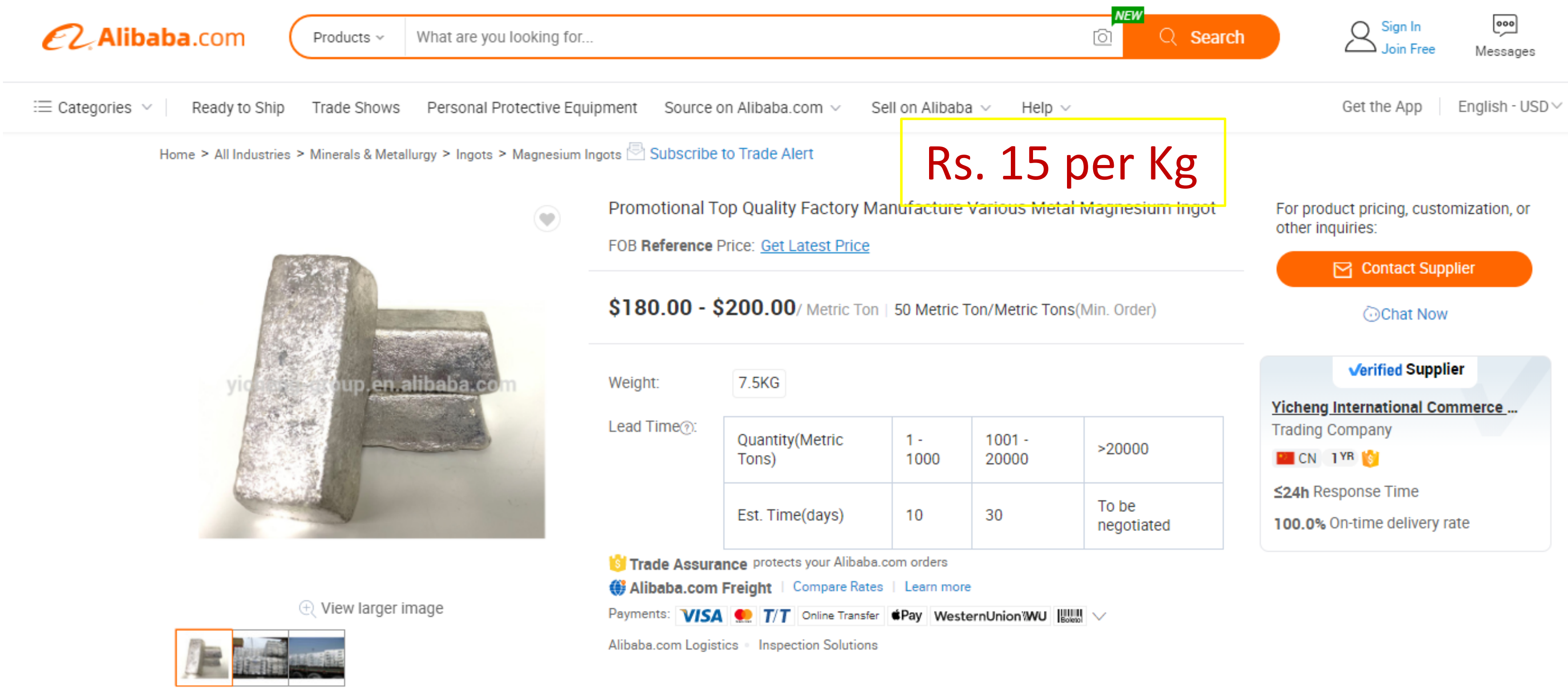
Rs. 45 per Kg



Rs. 1 per Kg



Rs. 15 per Kg



Price ~ Rs. 700 per Kg (after powder)

Price of Mg Basic Carbonate (CAS Number: 39409-82-0)

https://www.sigmaaldrich.com

Product #	Description
13118	Magnesium carbonate basic, purum, light, ≥40% Mg (as MgO) basis, powder (light),

SKU-Pack Size	Availability	Pack Size	Price (INR)	Quantity
13118-1KG	Available to ship on 10.03.2021 - FROM	1 kg	2,100.05	0

Bulk orders? ADD TO CART

Product #	Description
63062	Magnesium carbonate basic, purum p.a., heavy, ≥40% (MgO),

SKU-Pack Size	Availability	Pack Size	Price (INR)	Quantity
63062-1KG	Available to ship on 10.03.2021 - FROM	1 kg	3,994.43	0

Bulk orders? ADD TO CART

Product #	Description
63032	Magnesium carbonate basic, tested according to Ph. Eur., heavy,

SKU-Pack Size	Availability	Pack Size	Price (INR)	Quantity
63032-1KG-F	Estimated to ship on 22.03.2021 - FROM	1 kg	4,535.68	0

Bulk orders? ADD TO CART

Price for Magnesium Carbonate ~ Rs. 100 per Kg (not basic)

Price ~ Rs. 2000 per Kg

Looking for Experts as our Team Members

1. Reactor Design

(Batch to flow, pilot plant design)

2. Chemical Engineer

(Up-scalable Process Development, Process Flow Diagram, Stream Table, and Mass & Energy balance etc.)

3. LCA Analyst

(full cradle-to-grave LCA, Fully considered cost per tonne)

Please Contact: Prof. Vivek Polshettiwar
Emails:
polshettiwar@gmail.com
vivekpol@tifr.res.in

"The outcome of basic research must help in the development of commercial products and technology to help resolve India's societal challenges"

India can not continue ***importing oil, solar panels, batteries***

and

then in coming times

CO_2 Capture and Conversion Technologies, which is the future.

India imported 270 Million Metric Ton of **crude oil** valuing $120 billion in 2019-20.

India bought **batteries** worth $ 1.2 billion in 2019-20.

India imported **solar cells and modules** worth $1,180 mn from China in Apr-Dec FY20

AATMA-NIRBHAR
BHARAT

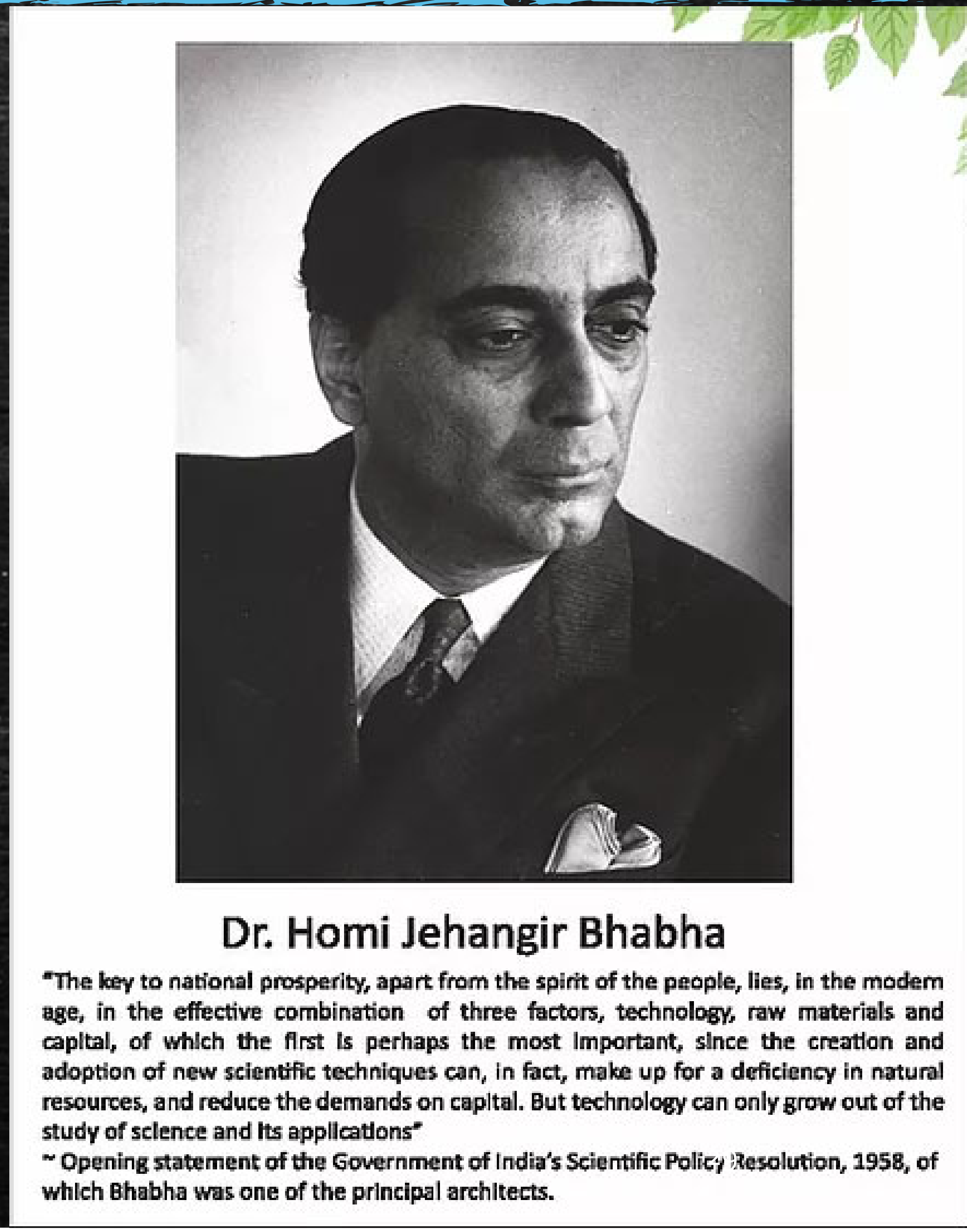
VISION of Dr. Homi J. Bhabha

Dr. Homi J. Bhabha, one of the chief architects of Government of India's Scientific Policy Resolution (1958), said

"The key to national prosperity, apart from the spirit of the people, lies in the modern age, in the effective combination of three factors: technology, raw material and capital, of which the first is perhaps the most important, since the creation and adoption of new scientific techniques can, in fact, make up for a deficiency in natural resources, and reduce the demands on capital. But **technology can only grow out of a study of science and its applications**."

Dr. Homi Bhabha built Department of Atomic Energy (DAE) and BARC and gave India Nuclear Power, the best example of Indigenous development and "Atmanirbhar Bharat".

Now it's time to harvest Solar Power and CO_2 for India's growth.



Funding

DAE

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Accelerating the Clean Energy Revolution
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Thank you !