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# 2D-NMs PHOTOCATALYST HYDROGEN EVOLUTION

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CLIMATE CHANGE – MAJOR PROBLEMS  
MITIGATING CO<sub>2</sub> EMISSION & RENEWABLE FUEL

Reduce **CO<sub>2</sub> Emissions**

Conversion into **Fuels/Chemicals,**

**Produce H<sub>2</sub> - Photocatalytic Conversion**

**Efficient & Affordable Photocatalysts**

**A Necessary – Development**

# WHY HYDROGEN FUEL?

S. No.	Fuel	MJ/Kg
1.	Liquid Hydrogen	130
2.	Aviation Gasoline	46.8
3.	Premium Gasoline/Petrol	46
4.	Regular Gasoline/Petrol	47
5.	Jet Fuel (Kerosene)	47
6.	Jet Fuel (Naphtha)	46.6
7.	Diesel	48
8.	Biodiesel	39.9
9.	Liquefied Natural Gas	55
10.	E85 (85:15:: ethanol : gasoline)	~33
11.	Ethanol	31.1
12.	Methanol	19.9
13.	Vegetable Oil	37.7
14.	Gasohol (10:90:: ethanol : gasoline)	~45
15.	Liquid Petroleum Gas (LPG)	~51



**Exploring  
2D-Nanomaterials ?  
Adjustable Charge  
Carrier Transport  
Carrier Lifetime...**

# OPTIMAL PHOTOCATALYST

Appropriate Band-Gap **Semiconductor**

Right Positioning – CONDUCTION/VALENCE Band

Satisfying – REDOX (**Reduction & Oxidation**)

CB/VB – More -ve/+ve – H<sub>2</sub>O Redox Potential

ENERGY BG  $\geq 1.23$  eV – H<sub>2</sub>O Split - H<sub>2</sub> and O<sub>2</sub>



# PHOTOCATALYTIC WATER-SPLIT

$h\nu \longrightarrow$  Chemical Energy



Efficiency – Semiconductor Band Structure

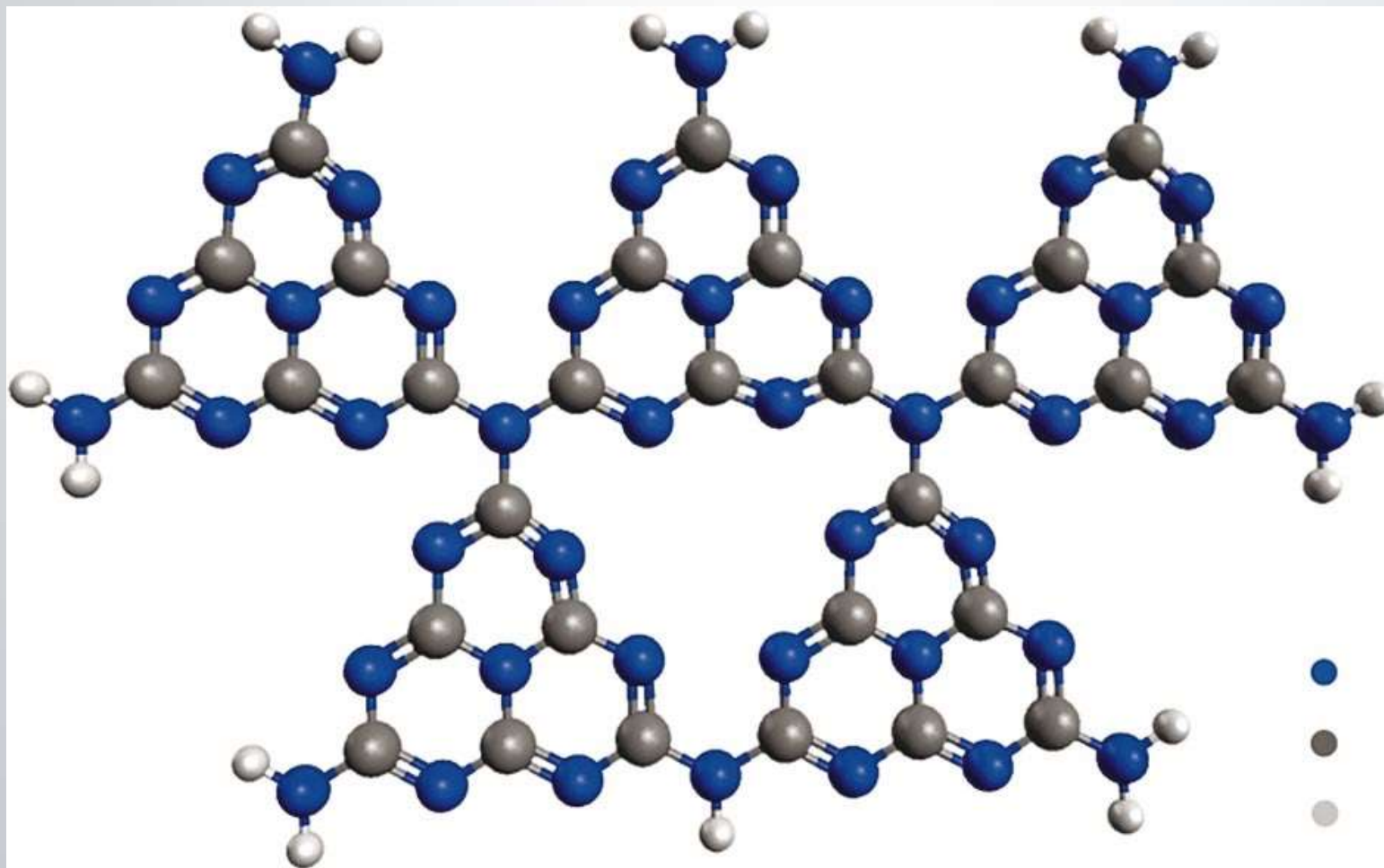
Efficient  $\text{H}_2$  production - Visible-light-driven

**Semiconductors - Bandgap - 1.23–3.0 eV**

# TWO-DIMENSIONAL NANOMATERIALS

- Since Discovery of **Graphene** from **Graphite**  
Exploration of **2D-NMs** Intensified
- Planar (Graphene), Quasi-planar Other NSs  
Form Family of Designer's Nanomaterials  
Programmable **Structure/Energy Band Gaps**

# G-C<sub>3</sub>N<sub>4</sub> GRAPHITIC CARBON NITRIDE

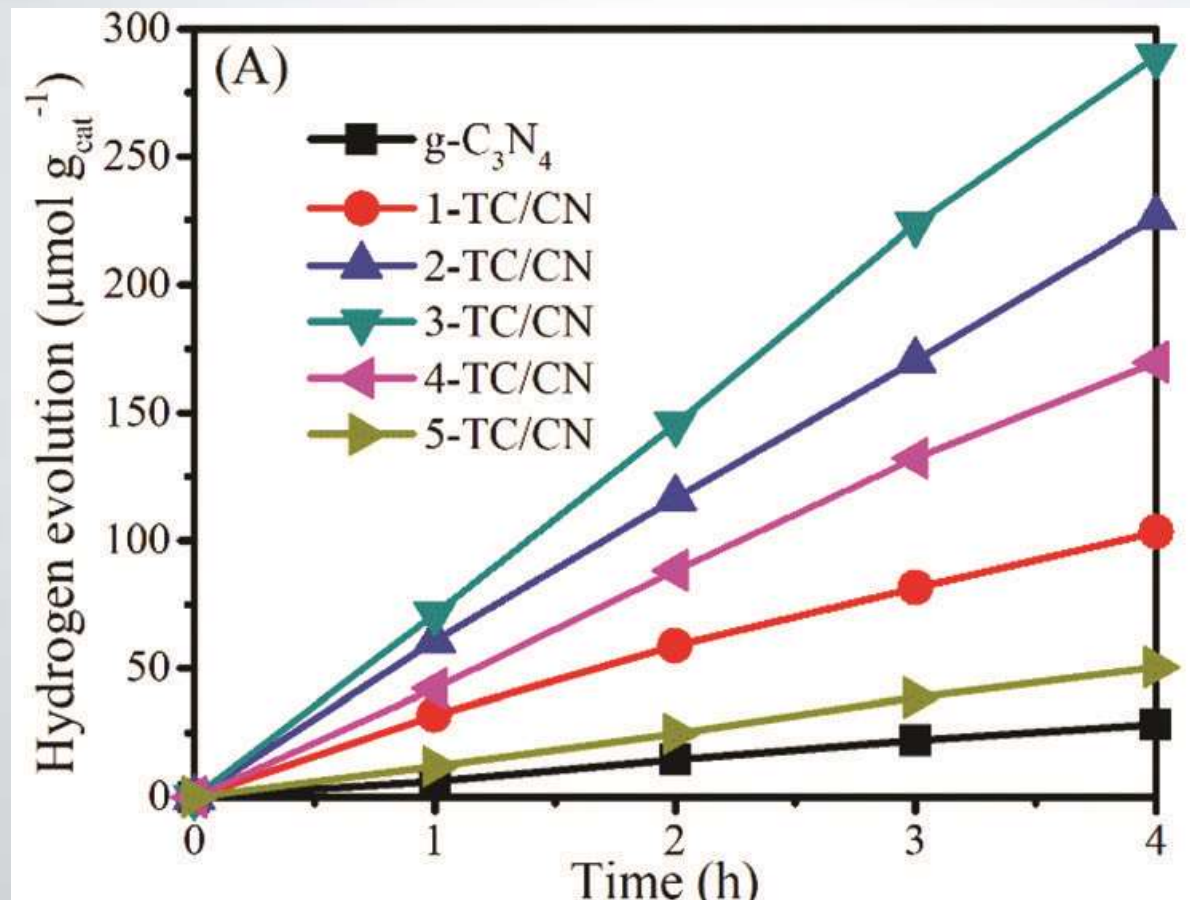




# G-C<sub>3</sub>N<sub>4</sub>-HETEROSTRUCTURE - PROBLEMS

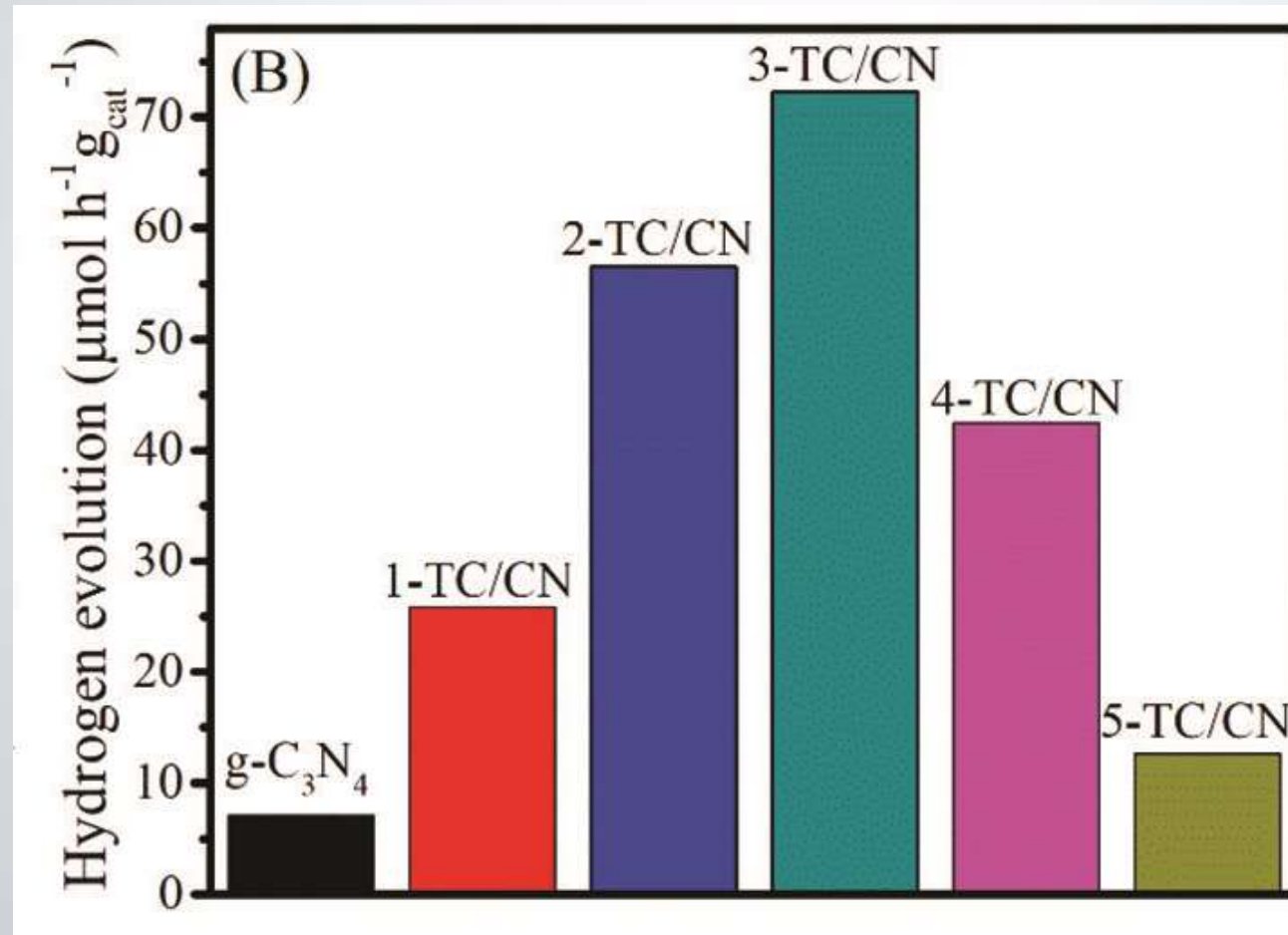
- Design of Band Structure Alignment
- Positioning for REDOX Reaction
- Enhancement of Efficiency
- Cost Effective Precursors

# COMPRARISION OF HYDROGEN EVOLUTION

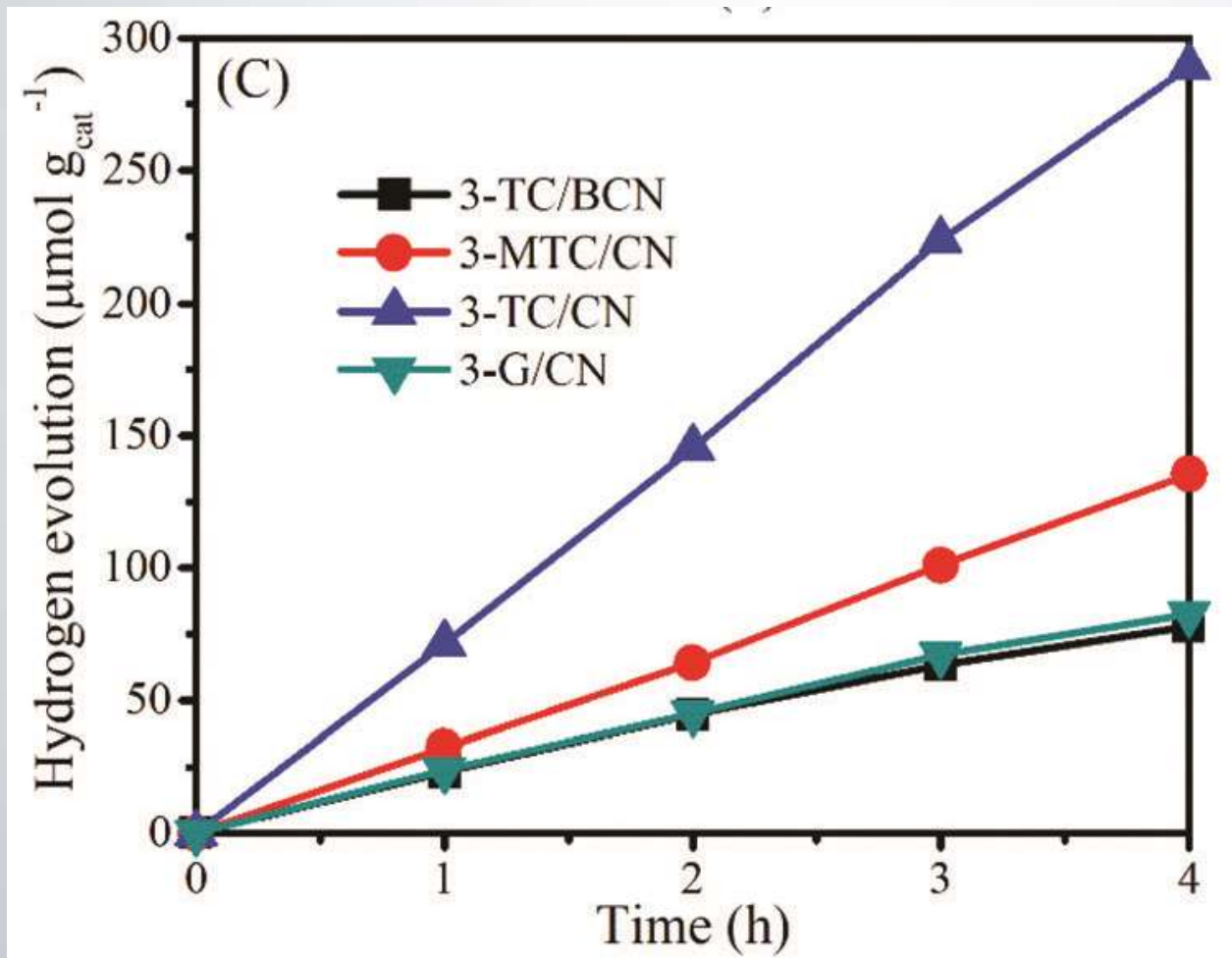


TC -  $\text{Ti}_3\text{C}_2$   
CN -  $\text{g-C}_3\text{N}_4$

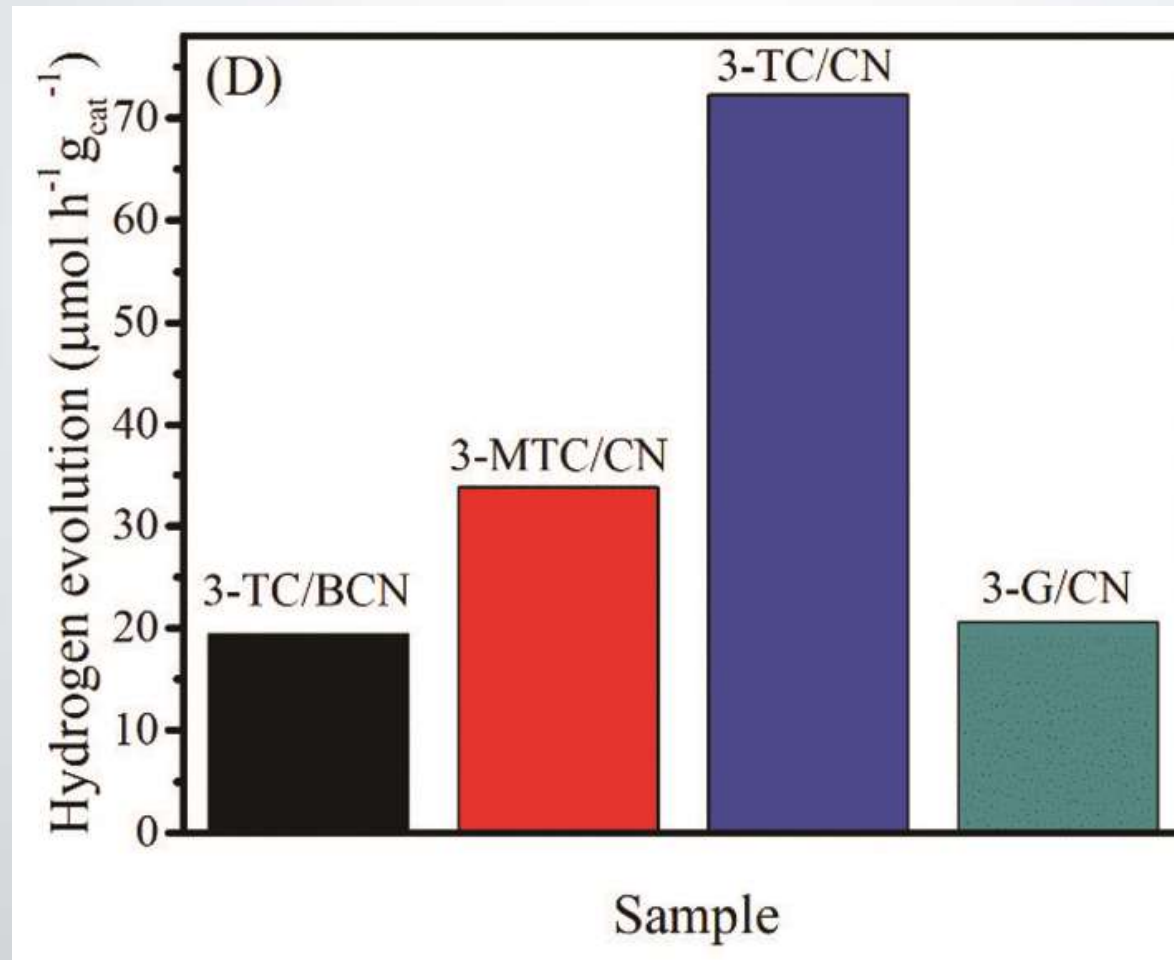
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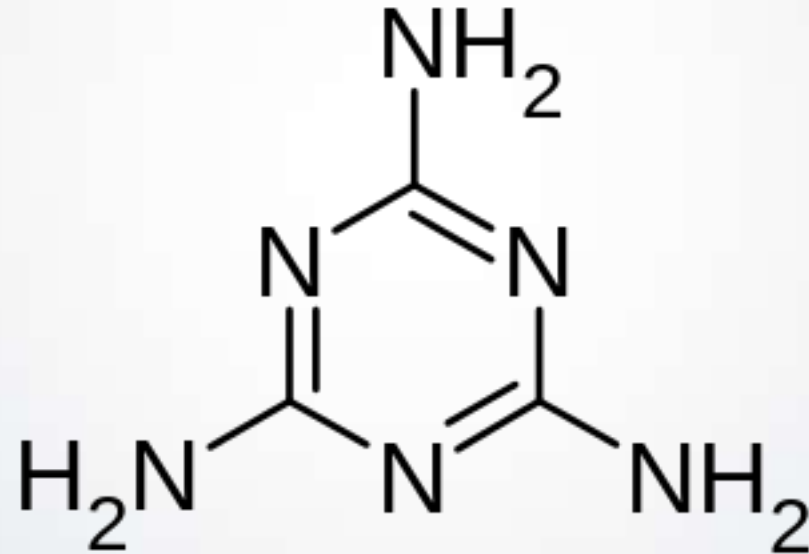
# COMPRARISION OF HYDROGEN EVOLUTION



# COMPRARISION OF HYDROGEN EVOLUTION



# MELAMINE - PRECURSOR

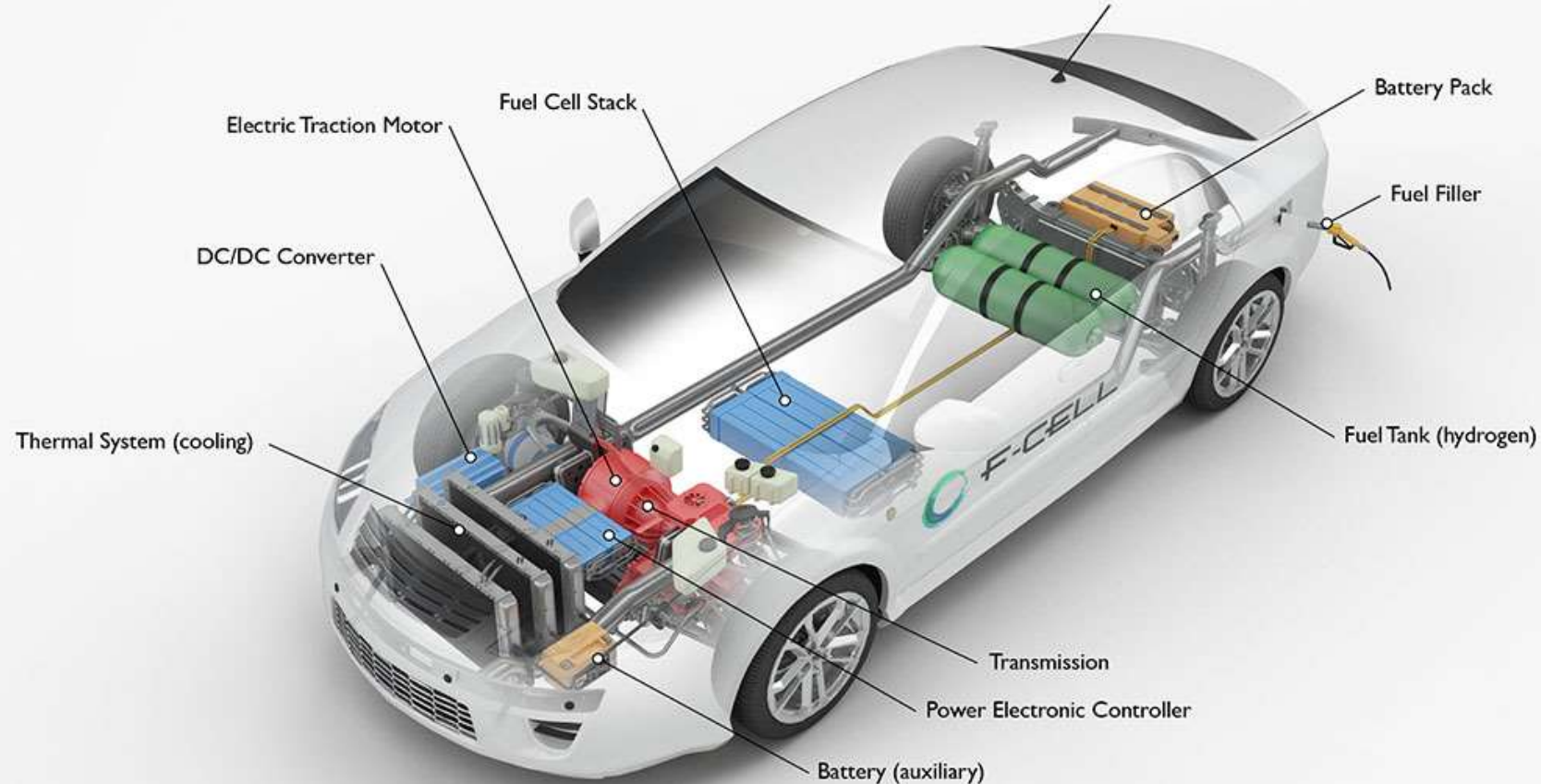


# DESIGN OF HETEROSTRUCTURES

- $\text{Cu}_2\text{O}/\text{g-C}_3\text{N}_4$  ,
- Graphene /  $\text{g-C}_3\text{N}_4$  ,
- $\text{CdS} / \text{gC}_3\text{N}_4$  ,
- $\text{TiO}_2 / \text{g-C}_3\text{N}_4$ .
- Untreated  $\text{g-C}_3\text{N}_4$  / Sulfidized  $\text{g-C}_3\text{N}_4$

# H<sub>2</sub> FUEL CELL POWERED CAR

Hydrogen Fuel Cell Vehicle





# CHALLENGES

- **Durability/Stability & Efficient Recycling**
- **Better Precursors – Critical Decision**
- **Newer Heterojunction & Homojunction – Needed**
- **Carbonaceous Semiconductors**

Metal and Non-metal Doping, Defects, and Interaction Mechanisms of Multiple Functions –  
**Optimal Hydrogen Production and Cost Effective Catalyst**

# CONCLUSIONS

2D–Semiconductor Nanosheets  
Appropriate Photocatalyst  
With Adjustable Parameters  
Rugged System Possible  
Right Kind of Precursor and  
Processing – Necessary  
Opportunities – Almost Unlimited