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Development of Two-dimensional Heterostructural Photocatalysts for Water Splitting Reaction

Yen Thi Hoang Le[123], Jeffrey C. S. Wu[12]

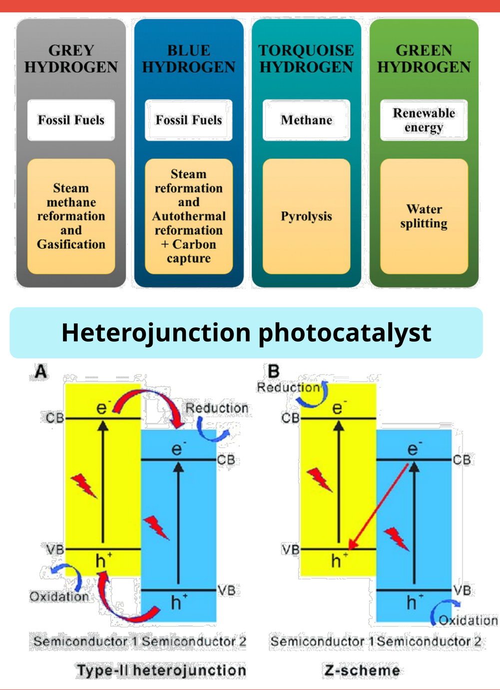
[1] Department of Chemical Engineering, National Taiwan University, Taipei, Taiwan

[2] Sustainable Chemical Science and Technology (SCST), Taiwan International Graduate Program (TIGP), Academia Sinica, Taipei, Taiwan

[3] Institute of Chemistry, Academia Sinica, Taipei, Taiwan

***Email**: Yen Le leyen0298@gmail.com, J.C.S. Wu cswu@ntu.edu.tw

Introduction

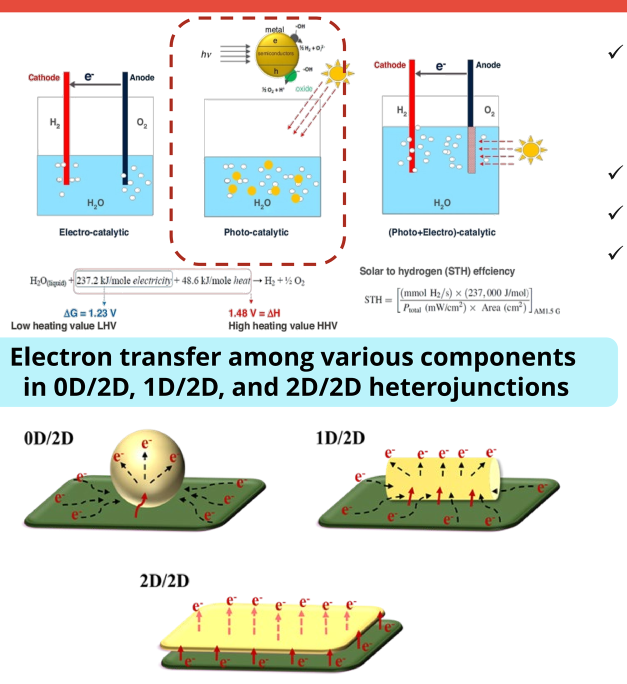


Pros: Simpler to design and synthesize; Easier to study

Cons: Poor charge separation; Limited redox power

Pros: Enhanced charge separation; Improved redox power

Cons: More complex design and synthesis

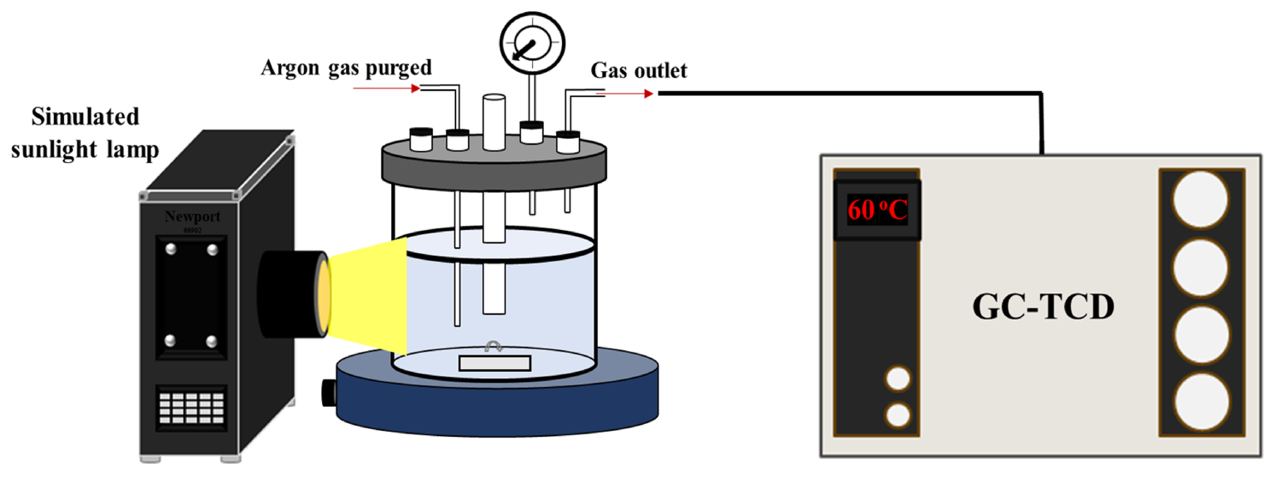


- ✓ Abundant and environmentally friendly resource
- ✓ Direct process
- ✓ Sustainable energy cycle
- ✓ Cost-effectiveness

2D/2D heterojunction brings many advantages, such as efficient charge separation, abundant light absorption, and the accessibility of numerous active sites.

Methodology

Photocatalytic water splitting set-up with simulated sunlight



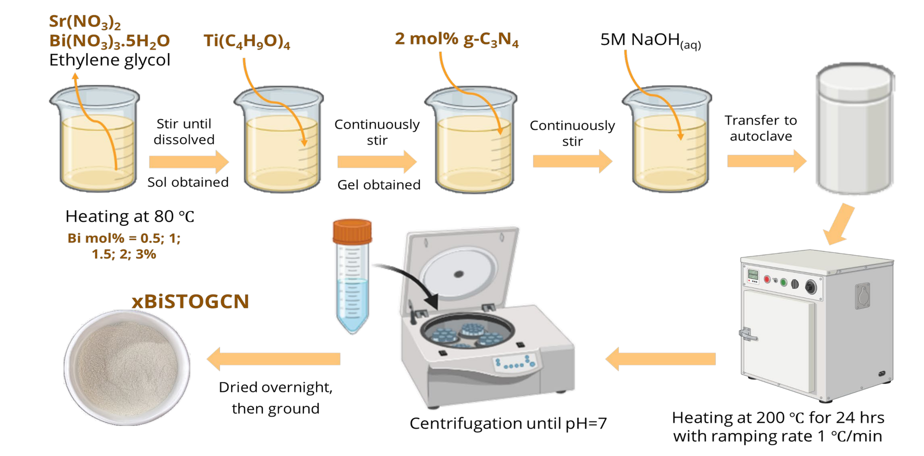
Noted: *The 200W UV light was also used for photodeposited Pt nanoparticles and some specific H_2 production reaction*

- ➢ 0.03 g of catalyst was dispersed in 100 mL of 10 vol% MeOH or DI water in a 310 mL quartz flask reactor
- ➢ Ar gas was purged for 20 mins
- ➢ 0.3 mL gas was detected every hour by GC-TCD, with Ar gas as a carrier gas
- ➢ A 300W Xenon lamp with the AM 1.5G filter

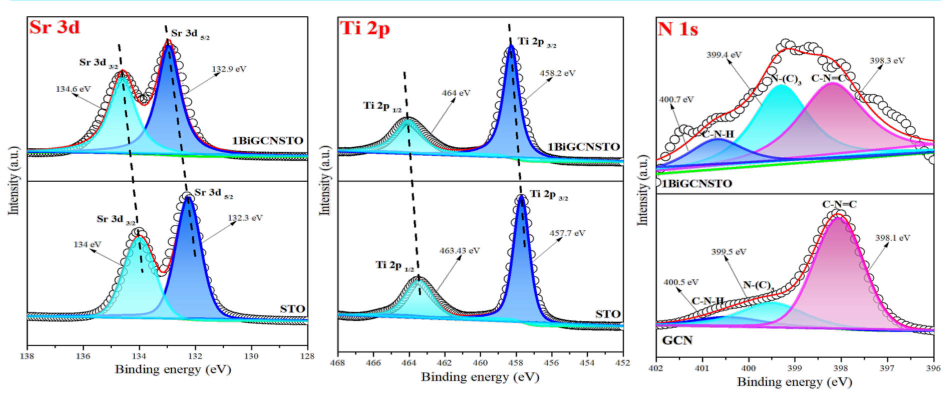
Results

Photocatalytic whole H_2O splitting using Bi^0-decorated $g\text{-}C_3N_4/SrTiO_3$ sheet-like catalyst under simulated sunlight

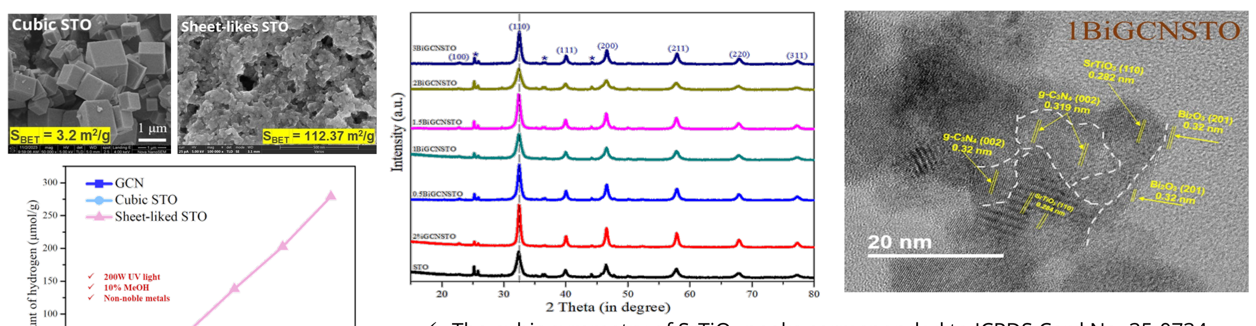
Photocatalyst synthesis procedure

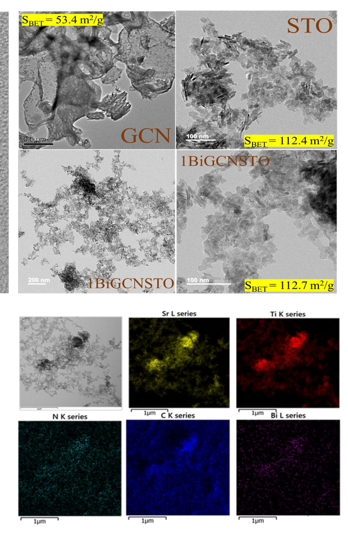


Electron transfer prediction



Crystallinity structure and morphology

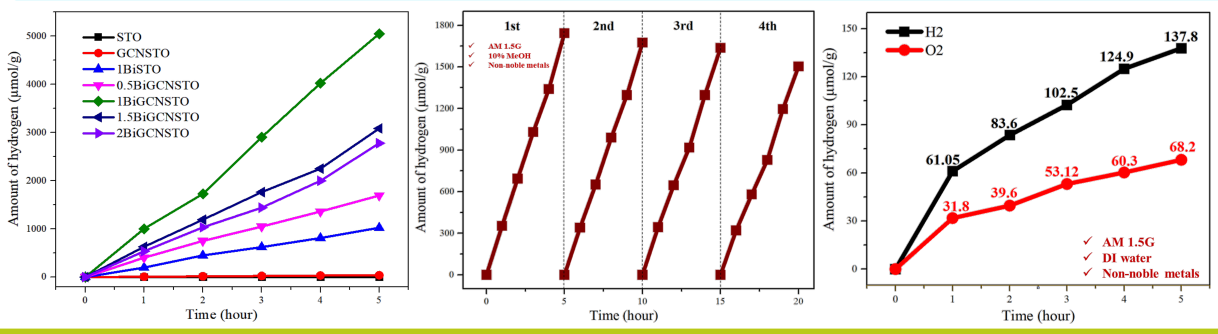




→ The contribution of ***high surface area*** → abundant active sites for easier accessibility of reactants, and enhances light absorption

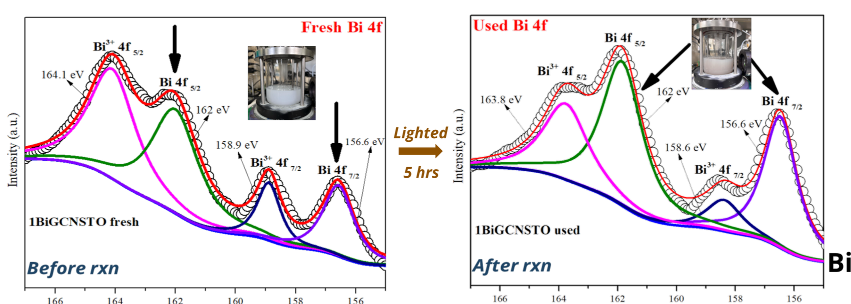
- ✓ The cubic symmetry of $SrTiO_3$ peaks corresponded to JCPDS Card No. 35-0734
- ✓ **The interface** of **GCN** and **STO**
- ✓ Very thin layer of Bi_2O_3 → **in-situ photoreduction** → Bi^0
- ✓ **Ethylene glycol** with hydroxyl groups → straightforwardly **adsorbed on STO (110)** → STO nanocrystals forming along the (110) crystal plane → ***sheet-liked morphology***

Photocatalytic water splitting reaction for H_2 production



- ✓ At ***1 mol% of Bi-added***, the highest H_2 evolution was obtained, **46-fold higher** than the samples without bismuth added
- ✓ Generated H_2 and O_2 **slightly decreased** due to the **backward reaction**

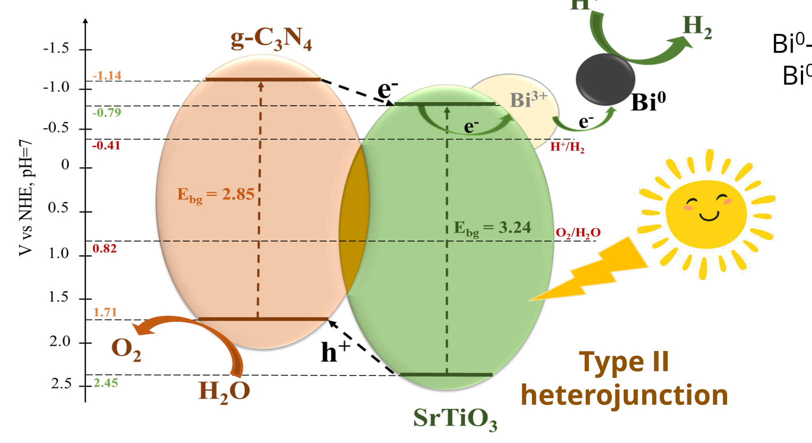
High resolution XPS of Bi 4f before and after photocatalytic rxn



The reason for the color change from white to greyish brown could be the formation of metallic bismuth

$Bi^{3+} + 3e^- \rightarrow Bi^0$ → Black in color

Possible mechanism for the overall water splitting reaction



$Bi^0 + H^+ + e^- \leftrightarrow Bi^0\text{-}H_{ads}$

$Bi^0\text{-}H_{ads} + B^0\text{-}H_{ads} \leftrightarrow 2Bi^0 + H_2$

$Bi^0\text{-}H_{ads} + H^+ + e^- \leftrightarrow Bi^0 + H_2$

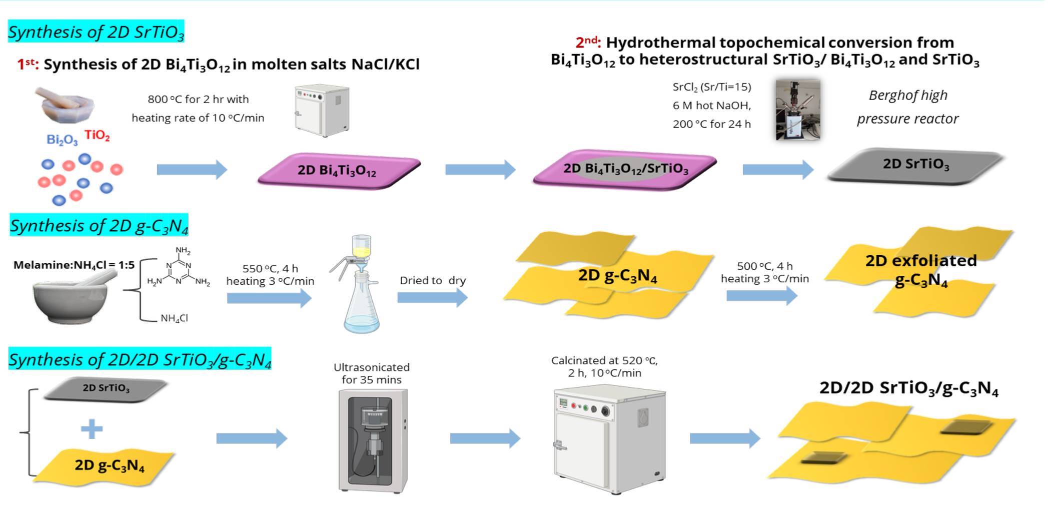
$H_2O + 2h^+ \leftrightarrow \frac{1}{2}O_2 + 2H^+$

→ e^- rapidly **migrated** to **Bi^{3+} sites** → **in-situ photoreduction** of Bi^{3+} to **Bi^0** → resulting **quickly reduced of water to H_2**

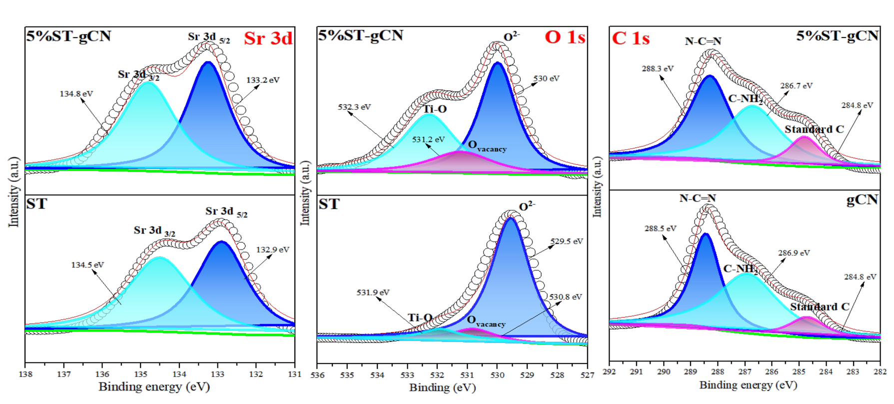
→ **Bi sites** served as **effective capture sites** and **active sites**

Distinctive 2-D $SrTiO_3/g\text{-}C_3N_4$ heterostructure photocatalyst for efficient photocatalytic water splitting reaction

Synthesis procedure, crystallinity structure, and morphology

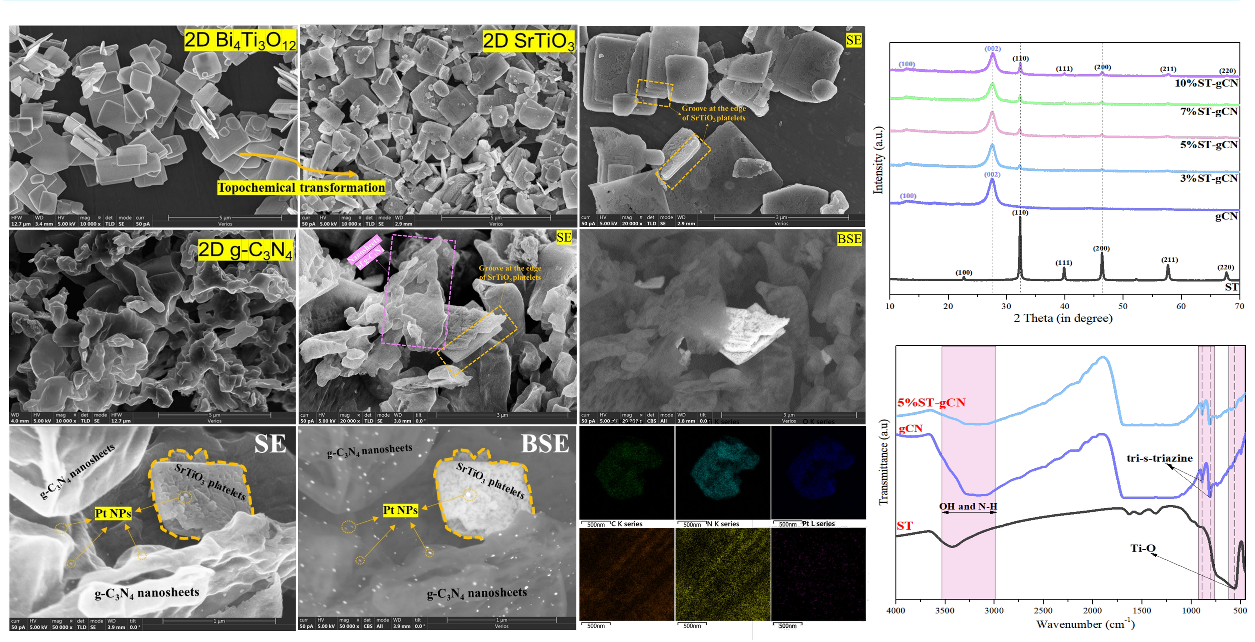


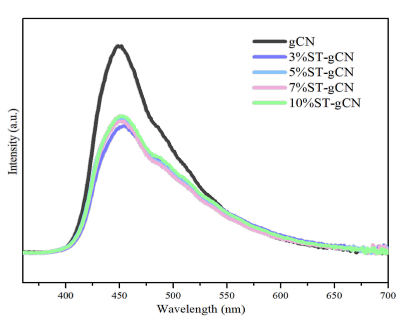
Electron transfer prediction



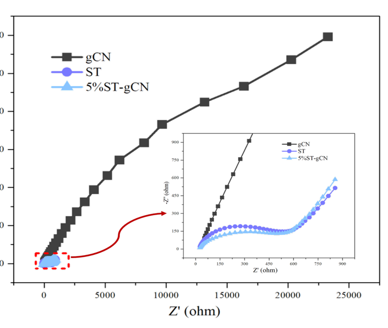
→ **Binding energies shifted** → **electrons** from **ST flowed** into the triazine rings of **gCN** between the **$SrTiO_3/g\text{-}C_3N_4$ interface**

Morphology, crystallinity, functional groups, and photo-electrochemical property



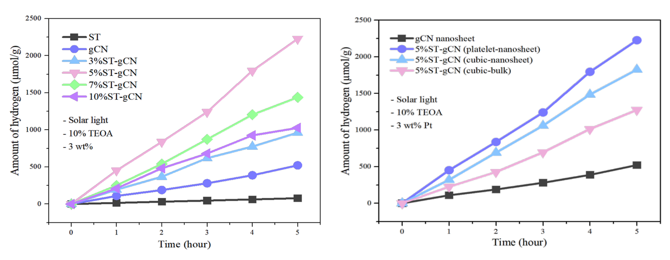


→ The **decreasing PL intensity improvement** of **interfacial charge transfer** between $g\text{-}C_3N_4$ and $SrTiO_3$

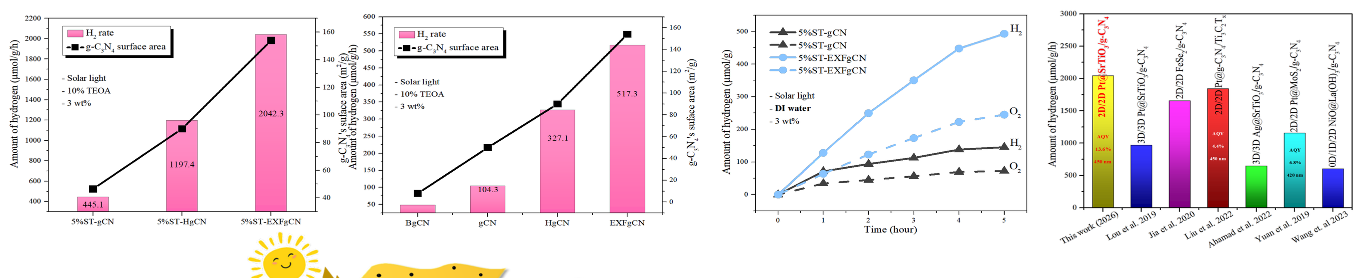


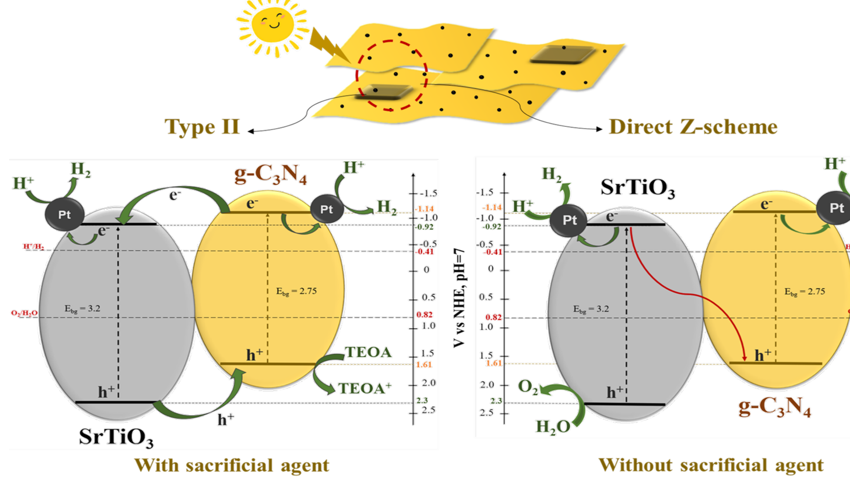
→ The curve radius of 5%ST-gCN composite is smaller than that of $g\text{-}C_3N_4$ → **reducing the transfer resistance**

Photocatalytic H_2 production reaction and possible mechanism



- ✓ **The optimal ratio of ST** for 2D heterojunction was **5 wt%**, which was 3-fold higher in H_2 production rate than pure gCN
- ✓ 2D/2D $SrTiO_3/g\text{-}C_3N_4$ heterostructure had the highest photocatalytic performance compared to bulk/cubic composites
- ✓ **5%ST-EXFgCN** exhibits the **highest H_2 production rate**, due to the greater surface area of EXFgCN, which enhances the 2D heterostructural formation, improves the light harvesting, and well-dispersed Pt nanoparticles





$gCN + hv \rightarrow gCN\ (e^- - h^+)$

$ST + hv \rightarrow ST\ (e^- - h^+)$

$gCN\ (e^- - h^+) + ST\ (e^- - h^+) \rightarrow gCN\ (e^-) + ST\ (h^+)$

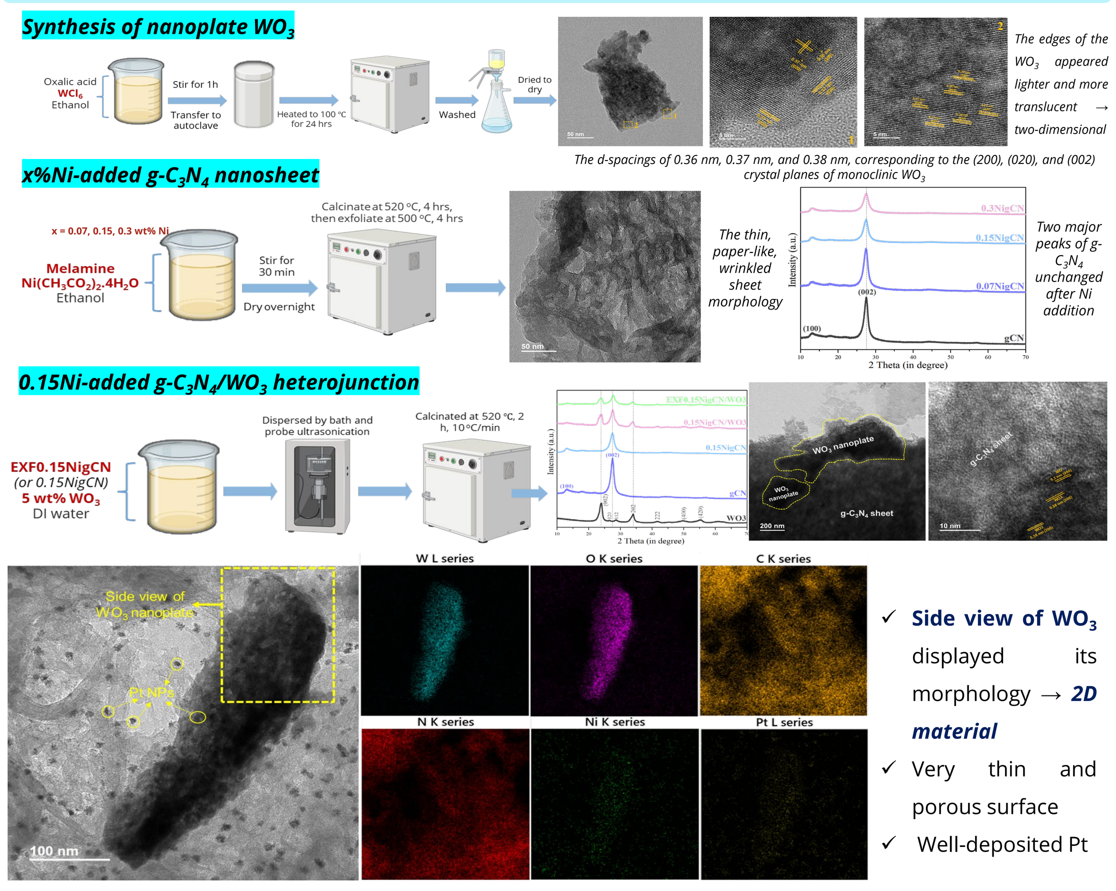
$2H^+ + 2e^- \rightarrow H_2$

$H_2O + 2h^+ \rightarrow \frac{1}{2}O_2 + 2H^+$

→ The possible mechanism was divided into 2 cases: ***with*** or ***without*** the presence of **TEOA** as a sacrificial agent

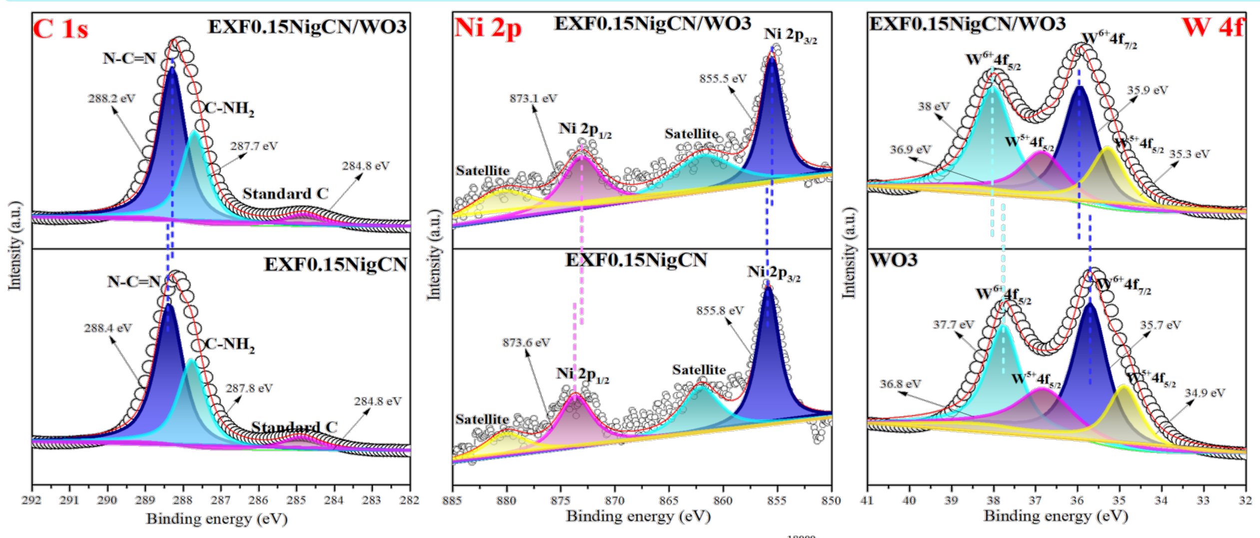
Development of Two-Dimensional Direct Z-Scheme $Ni(OH)_2$-decorated-$g\text{-}C_3N_4/WO_3$ Heterojunction Photocatalyst for Water Splitting Reaction

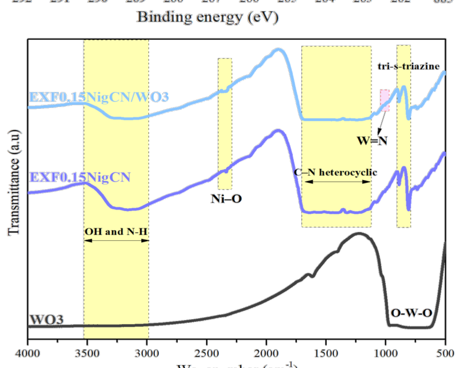
Photocatalyst synthesis procedure



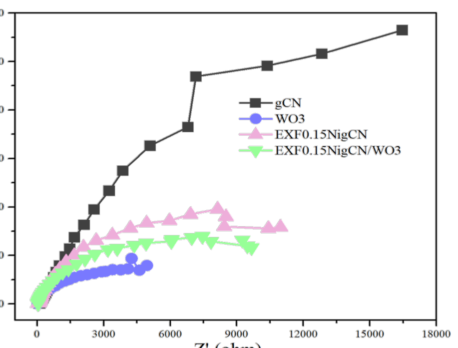
- ✓ **Side view of WO_3** displayed its morphology → ***2D material***
- ✓ Very thin and porous surface
- ✓ Well-deposited Pt

Electron transfer prediction, functional groups, and electrochemical property

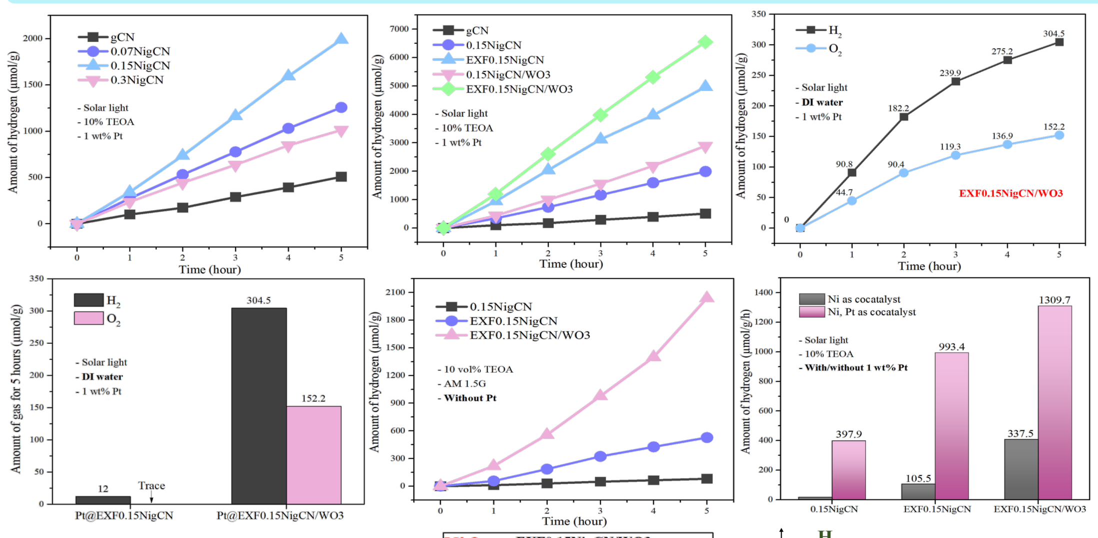




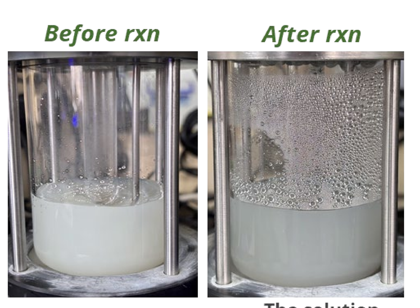
→ The new small peak at **972.2 cm^{-1}**, which can be ascribable to the **W–N bonds**, thus suggesting the **chemical connection formed** between modified-gCN and WO_3



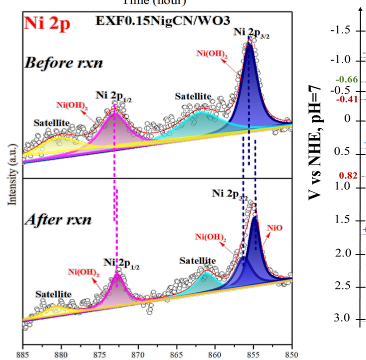
Photocatalytic H_2 production reaction and possible mechanism

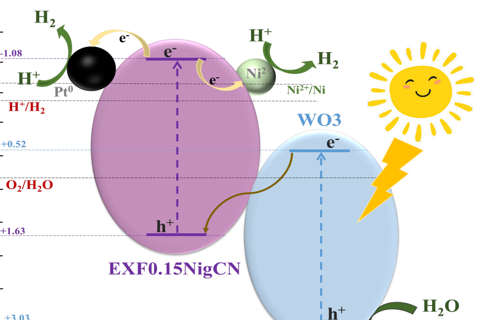


The **2D/2D EXF0.15NigCN/WO3** → enhancing the interfacial contact area through face-to-face contact between WO_3 nanoplates and EXF0.15NigCN nanosheets → **maximizing the probability of Z-scheme recombination**



$Ni^{2+} + 2e^- \rightarrow Ni^0$ → The solution color changed





→ The **$Ni(OH)_2$ partially reducing** Ni^{2+} to Ni^0 atoms → co-catalysts

Conclusion

- ✓ The study has successfully synthesized three kinds of heterojunction photocatalysts with two-dimensional morphology for efficient photocatalytic hydrogen production through the water splitting reaction under simulated sunlight
- ✓ The possible mechanism has also been reported

References

Le, et al. "Photocatalytic whole H_2O splitting using Bi^0-decorated $g\text{-}C_3N_4/SrTiO_3$ sheet-like catalyst under simulated sunlight." International Journal of Hydrogen Energy 130 (2025): 390-401.

Le, et al. "Distinctive 2-D SrTiO3/g-C3N4 heterostructure photocatalyst for efficient photocatalytic water splitting reaction." Solar Energy Materials and Solar Cells 303 (2026): 114389.

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