

2D C-N Semiconductors: Earth-Abundant Photocatalysts with Tunable Bandgaps

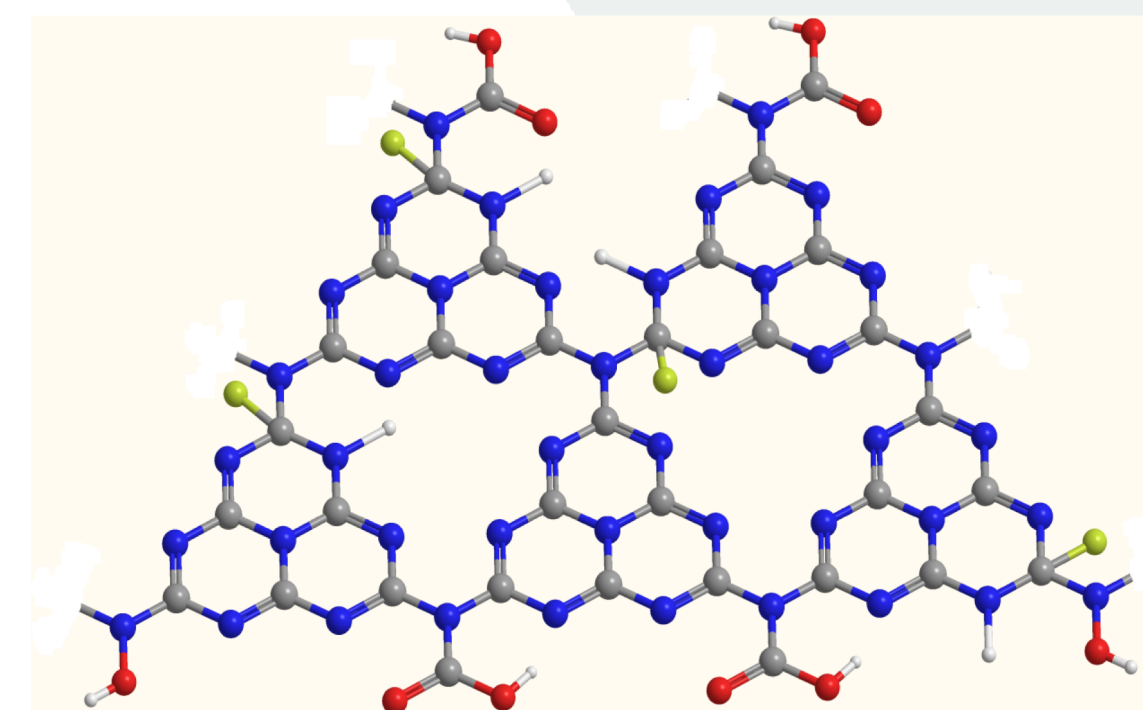
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BACKGROUND

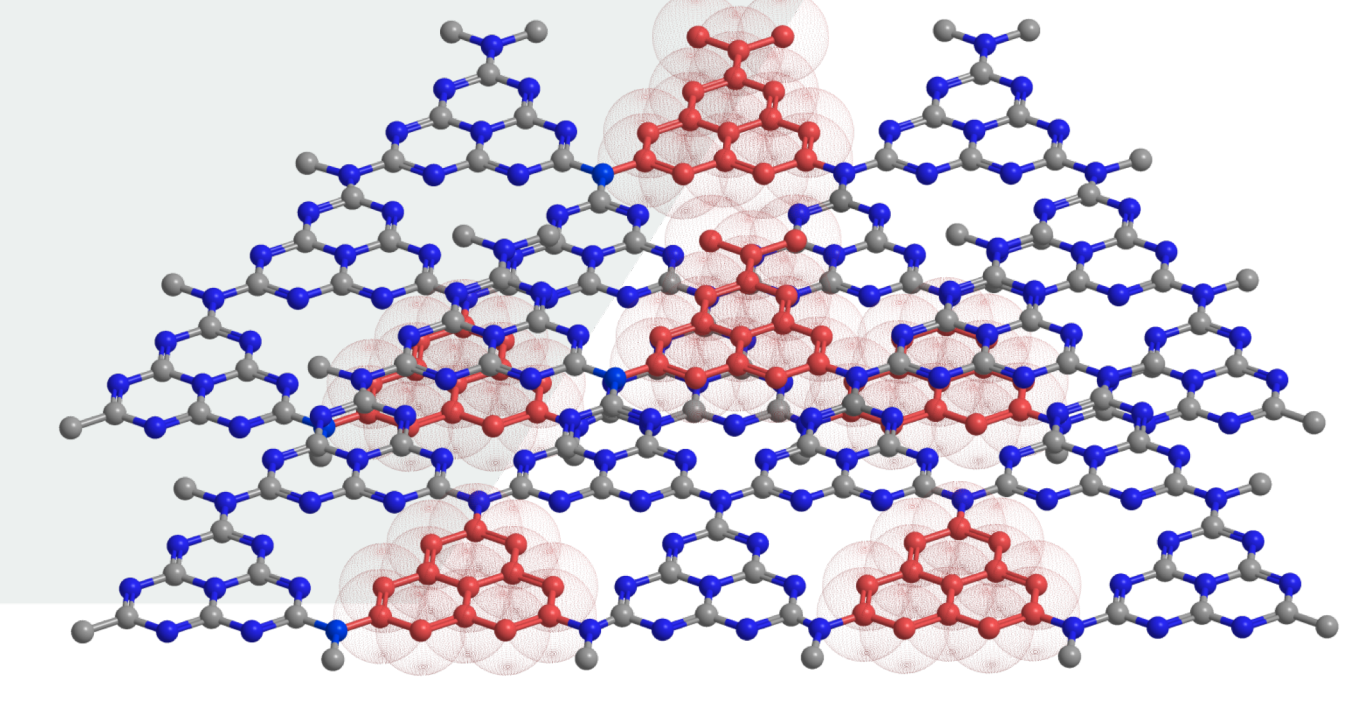
To function as an efficient and durable photocatalyst, a semiconductor nanomaterial has to have adequately long carrier lifetimes, be resilient to harsh chemical environments, resist catalyst poisoning or allow for easy regeneration, and harvest a broad spectrum of photons in sunlight, ranging from the ultraviolet to the near-infrared. In addition, large scale commercial deployment of photocatalysts requires the active materials to be non-toxic, earth abundant and easily processable. The single biggest problem facing the field of photocatalysis is that the aforementioned requirements conflict with each other for nearly every available semiconductor. In this context, graphitic 2D semiconductors containing a core of carbon and nitrogen atoms offer an exciting way forward, since members of this family have tunable band gaps, are cheap, chemically resilient, and also have excellent electronic parameters. In the Shankar Lab, we have synthesized a variety of new C-N containing 2D semiconductors in the form of both bulk material (powders and films) and quantum dots. The developed photocatalytic systems exhibit excellent photoresponse under visible light irradiation for various applications *i.e.* water splitting, pollutant degradation and CO₂ reduction.

AIMS AND OBJECTIVES

- We have prepared chemical and photostable visible light active CN quantum dots and bulk CN sheets by nanoscale modification in chemical structure of heptazine unit and doping with various hetero atoms such as P, F *etc.*
- The band gap/band structure of CN quantum dots/nanosheets can be manipulated to **desired** position by controlling degree of chemical and compositional change.
- CN quantum dots integrated with TiO₂ nanorods by *in situ* approach, and bulk CN sheets show promising outcomes in photoelectrochemical water splitting under visible light irradiation.

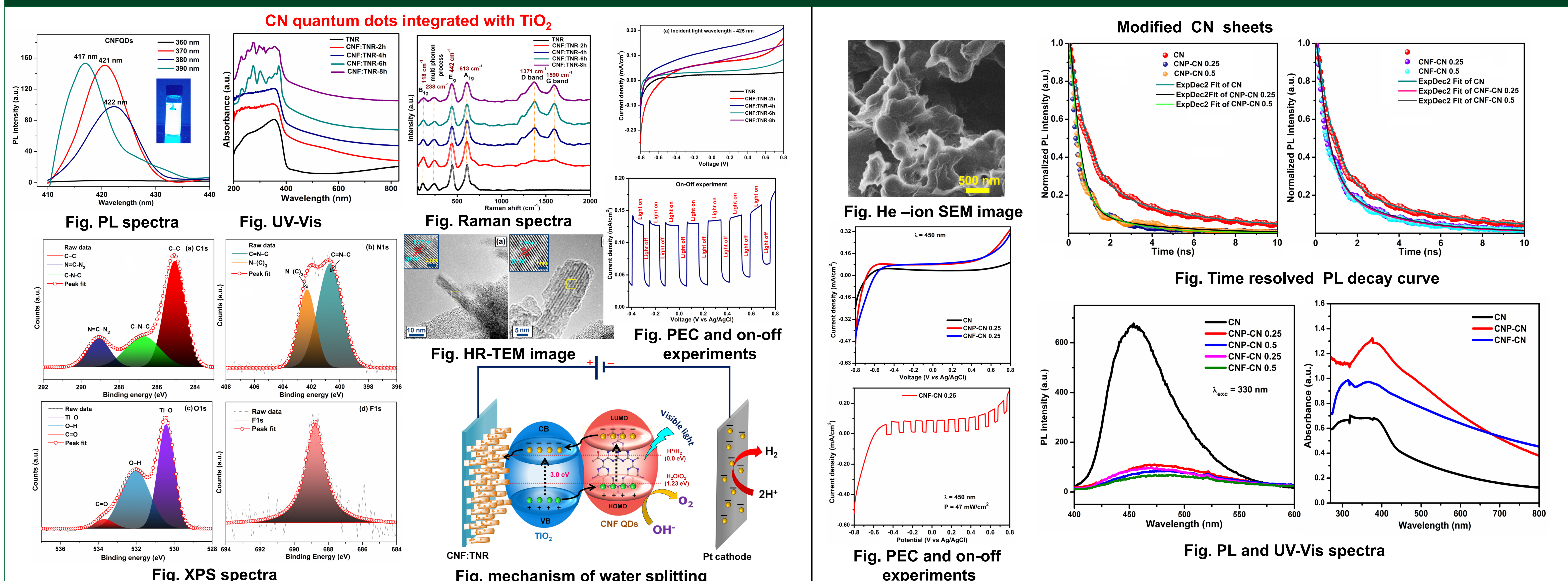


CN quantum dots



Modified CN sheets

RESULTS



FUTURE DIRECTIONS

- New CN materials will be prepared by introducing different units in the scaffold of CN sheets.
- Compositional and optical properties will be determined by various tools.
- Hybrids of 2D CN sheets and various semiconductors/and or inorganic 2D sheets will be designed for the photocatalytic applications
- CN quantum dots will be introduced in various photocatalytic systems to harvest maximum part of solar spectrum
- Developed materials will be tested for various photocatalytic applications such as hydrogen evolution, solar cells, CO₂ reduction, dye degradation *etc.*

PARTNERS

Technical University of Munich (NSERC Create Grant): We are working with the Thomas Nilges Group on new visible absorbing semiconductors, and with the Müller-Buschbaum group on new solar energy harvesting configurations.
University of Bayreuth: The Panzer group is testing fundamental optoelectronic properties of our halide perovskite single crystals.
NRC-NINT: We are actively collaborating with Drs. Alex Kobryn and Sergey Gusarov on DFT, MD and RISM modeling of TiO₂-based and perovskite-based nanomaterials.
UofA Chemistry: Dr. Guy Bernard and Prof. Vlad Michaelis are assisting us in solid-state NMR studies of newly synthesized graphenic semiconductors

FES PROJECT OVERVIEW

T12:P02 Artificial Photosynthesis Using Semiconductor Nanomaterials

The research presented in this poster explores noble metal-free, earth abundant nanomaterials as new visible light absorbing, photostable semiconductors, not merely for CO₂ photoreduction but also relevant to the broader FES theme of solar energy harvesting, which includes materials genomics, sunlight-driven water-splitting and solar cells. The key insight here is that graphenic semiconductors (e.g. carbon nitride) present a family of 2D-thin film and quantum dot semiconductors with high carrier mobilities, large active surface areas, earth-abundance, high carrier mobilities and tunable bandgaps. Graphenic semiconductors frequently require an electron transporting scaffold that provides a percolating network for carriers. Hence, we have started to integrate graphenic semiconductors with one-dimensional TiO₂ nanostructures (nanorods, nanotubes) to form visible light-active photocatalysts.

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FUTURE ENERGY SYSTEMS



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