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An insight into band-bending mechanism of Cu-based NPs with dynamic charge transfer for photocatalysis applications

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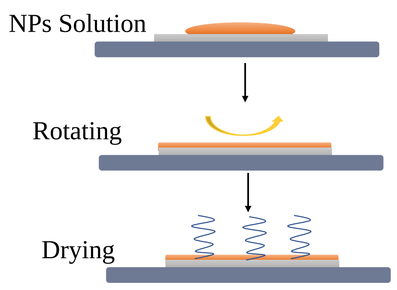
Introduction & Methods

A significant amount of toxic waste including dyes is discharged into aqueous bodies, requiring immediate solutions from scientific communities. Photocatalysis is the most promising method being explored for the degradation of effluents in recent years and is considered as a green route for environmental remediation.

- In this work, we synthesized Cu-based nanoparticles (NPs) in a one-step via a non-aqueous sol-gel method for visible-light photocatalytic degradation of Neutral red (NR) dye.
- The photocatalytic activity of Cu-based NPs originates from the band-bending leading to electron transfer at the metal-semiconductor interface and the production of Reactive Oxygen Species (ROS).
- The as-synthesized photocatalytic NPs were also deposited on glass substrates for easy recovery and reusability by spin coating.

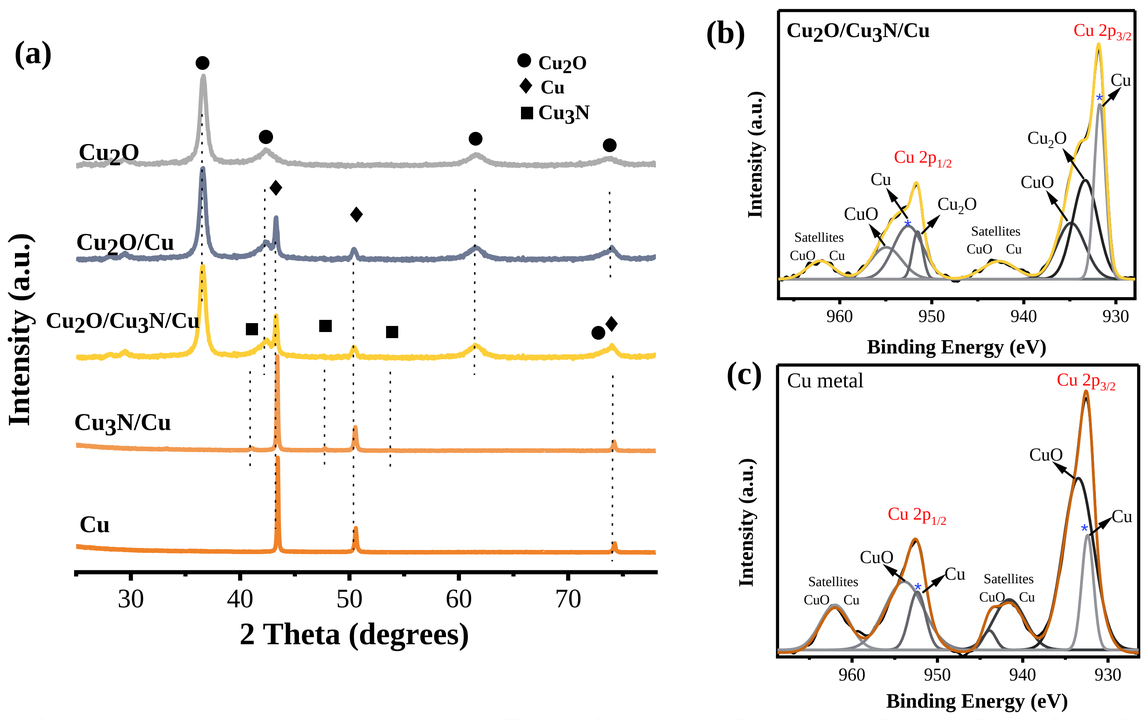
Thin films deposition by Spin coating Process



Spin coated films on glass substrate

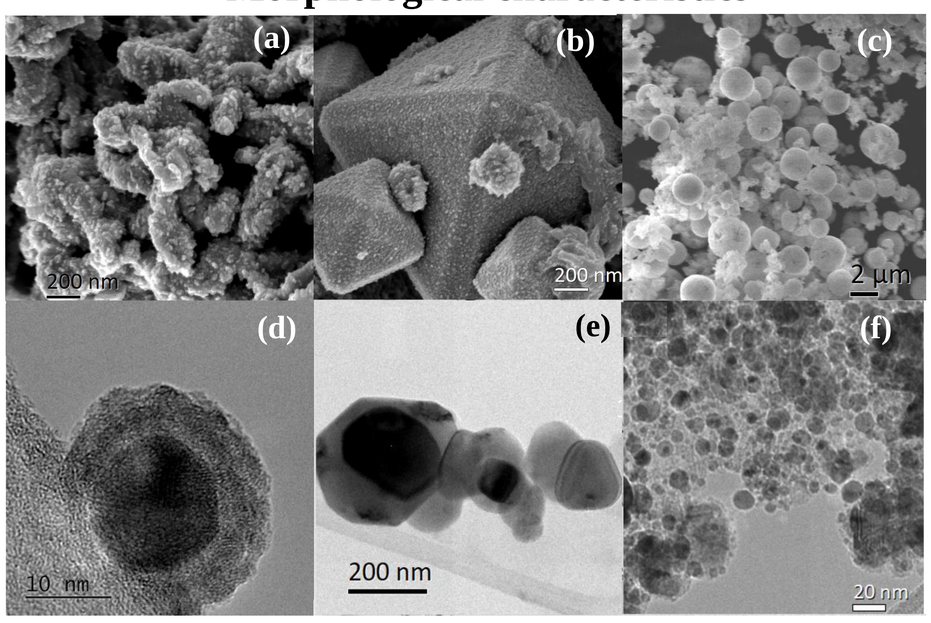
Nanomaterials Characterization

Structural and Chemical Characterization



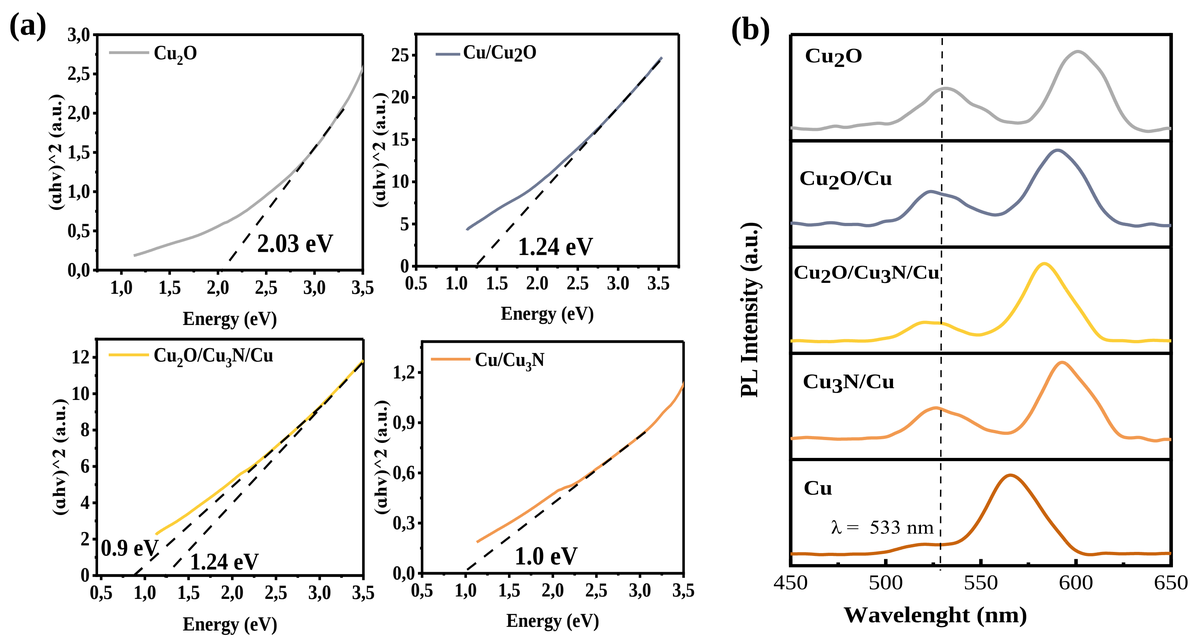
(a) The XRD patterns indicate crystalline phases of the as-synthesized Cu-based NPs. The XPS spectra of Cu2p of (b) $Cu/Cu_2O/Cu_3N$ and (c) Cu metal NPs confirm the surface chemical composition of the photocatalysts.

Morphological characteristics



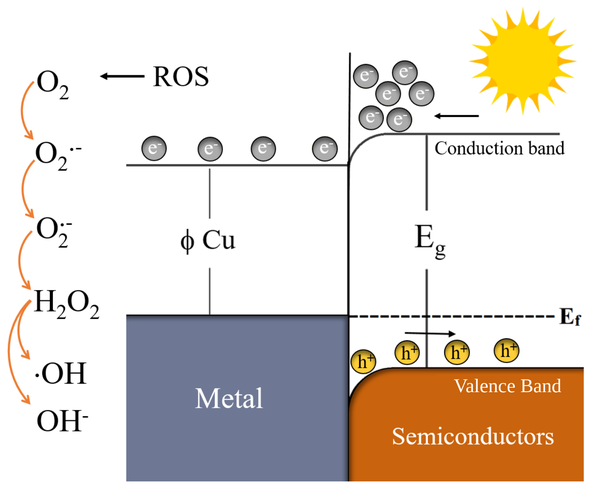
(a-c) SEM micrographs of Cu, Cu/Cu_2O and Cu/Cu_2O NPs, respectively. (d-f) TEM micrographs of Cu_2O NPs, Cu/Cu_2O and Cu NPs respectively.

Optical Properties



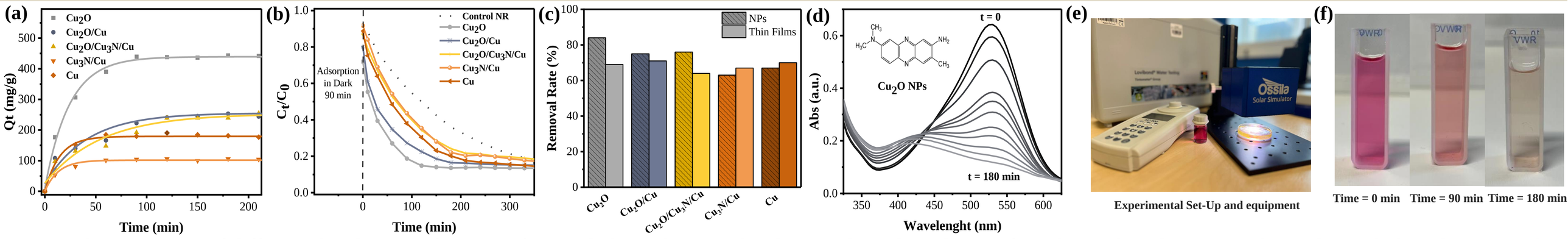
(a) Band gaps of the nanoparticles were determined from Tauc Plot.s calculated using UV-Vis absorption spectra., indicating that all samples have a high capacity of visible light absorption. (b) The PL spectra show the changes in the emission peak positions that can be attributed to electron transfer mechanisms between the various phases as well as changes in radiative recombination influenced by semiconductor band bending.

Photocatalytic Mechanism



The presence of the plasmonic Cu metal NPs induces downward band bending in the p-type semiconductors, creating electron accumulation on their surfaces and preventing the excitonic recombination of the e^-/h^+ pairs in Cu_3N or Cu_2O. The accumulation of electrons on the nanoparticle surface supports the photocatalytic mechanism based on the generation of ROS on the transfer of electrons from the nanoparticle surface to the oxygen and hydroxyl radicals present in the aqueous medium.

Photocatalytic Degradation Studies



(a) NR adsorption (Qt) of different absorbents as function of time (dark conditions), (b) photocatalytic degradation of NR by Cu-based nanoparticles under sunlight radiation, (c) bar graphs comparison of NR degradation efficiency using NPs and thin films, (d) UV-vis absorption spectra of NR from 0 to 180 min of photocatalytic reaction by Cu_2O NPs, (e) experimental setup of the photocatalytic source and (f) photographs of the dyes after several intervals of dye degradation.

Conclusions

- In this study, the non-aqueous sol-gel method was developed to synthesize Cu-based nanostructures for optimal photocatalytic activity.
- Cu-based NPs were deposited on glass substrates for easy recovery of the NPs after use.
- The band-bending, mechanisms is instrumental in the photocatalytic activity of the semiconductor NPs with plasmonic Cu metal NPs for ROS production.

Acknowledgments

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References

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