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Titania-based Metal Photo-catalysts for Organophosphate Neutralization

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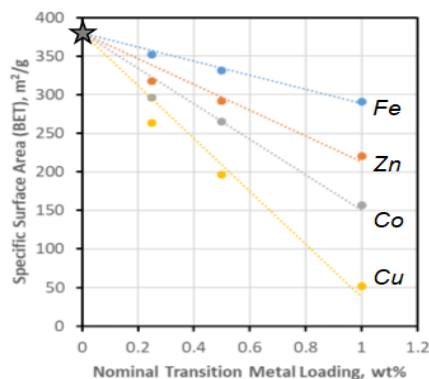
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Katelyn Alley (BS Chem '21), Quinn Cunneen (BS Chem '20) and Dario Prieto

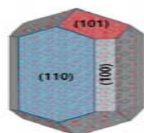
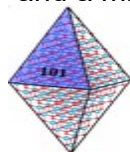
Background & Significance

- Organophosphates (OP) inhibit the breakdown of neurotransmitters and are extremely toxic
- Silica-supported metal catalysts can neutralize OP in presence of H_2O_2
- H_2O_2 is hazardous to transport, unsustainable to produce
- Silica decomposes during synthesis



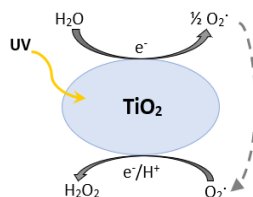
Potential solution: Titania

- Robust porous oxide with high SSA
- Two crystal phases (Rutile, Anatase) and a mixed phase (Aeroxide)



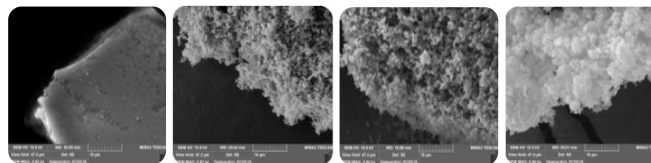
From: Illas et al. J. Phys. Chem. Lett. 2017, 8, 22, 5593

- H_2O_2 production under a UV irradiation



Adapted from: Catal. Sci. Technol. Royal society of chem, 7 (2017), 4977-4983

Higher metal loadings with Titania



Silica Anatase Rutile Aeroxide

Incipient Wetness, ml/g

0.7 0.4 0.4 **0.8**

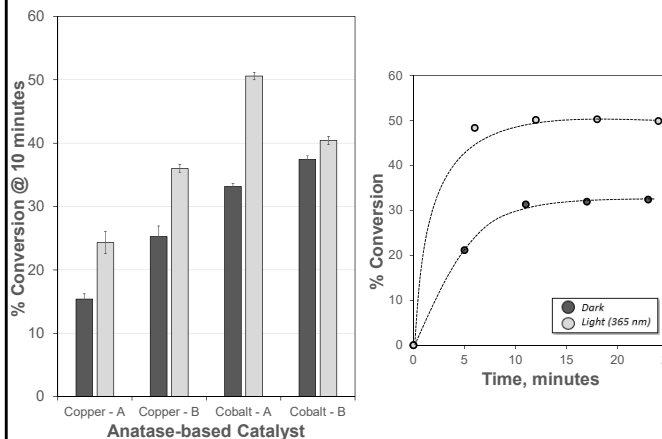
Surface Area, m²/g

370 50 50 65

Metal loadings, atom/nm²

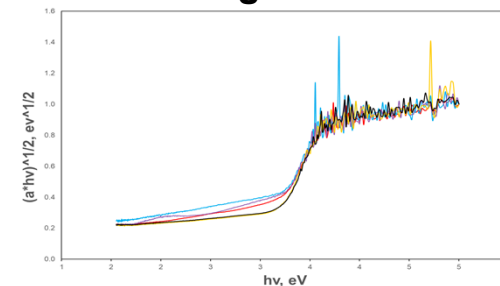
0.00076 0.0032 0.0032 **0.0049**

UV light increases the rate of reaction



- Reaction can occur without UV light but the addition of UV light increases the reaction rate
- Materials prepared with EDTA and Nitrate show same reactivity
- Addition of titania to silica-based catalysts increases the reactivity

Metal loading affects activity



- The photoactive properties remain constant regardless of the material
- Activity change is due to the metal

Conclusion

- The materials are active in organophosphate neutralization without an oxidant
- No obvious changes in the band gap
- Light increases reaction
- The catalysts deactivate

Upcoming work

- Extend method to Fe, Co, and Zn
- Effect of metal precursor and loading on surface area and metal structure

Acknowledgments

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Katelyn Alley Biochemistry 21'



I am currently a junior at Montana Technological University pursuing my degree in Biochemistry. I was born and raised in Butte, Montana and decided to pursue my degree at my hometown college. After graduation, I plan on pursuing a Ph.D. in chemistry. In the future, I would like to work as an educator to inspire the next generation of scientists.