Microscale Structure-Property Relationships and Antibacterial Activity of Microscale Fe-Doped ZnO

J. Brannon[1], Lexi Klements[2], Landon Davies[2], Melissa Remezo[3], Mikhail Quiroz[3], Parmeet Johdka[4], Alex Baumann[4], Louise Hutchison[1], Joshua Humphrey[1], Sam Tran[1], Garrett Shuler[1], Brian Mata Mata[1], Shauna McGillivray[1], Yuri Strzhemechny[1]

Texas Christian University[1]; Texas Academy of Biomedical Sciences[2]; Harmony School of Innovation Fort Worth[3]; Tarrant County College[4]

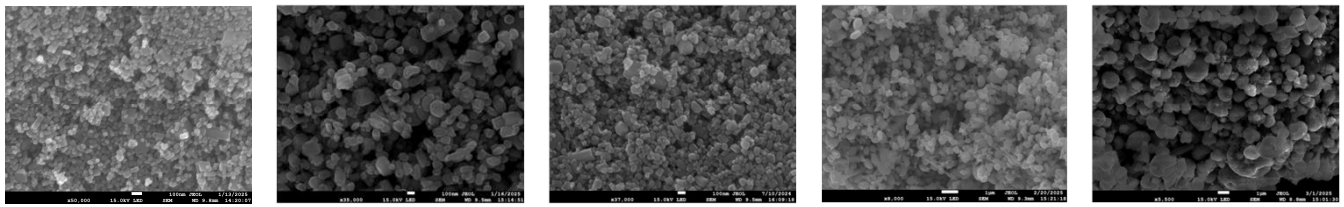
Concise Abstract/Introduction:

Key Idea: At the micro/nanoscale, ZnO behavior depends heavily on **surface structure, defects, and electronic surface states**.

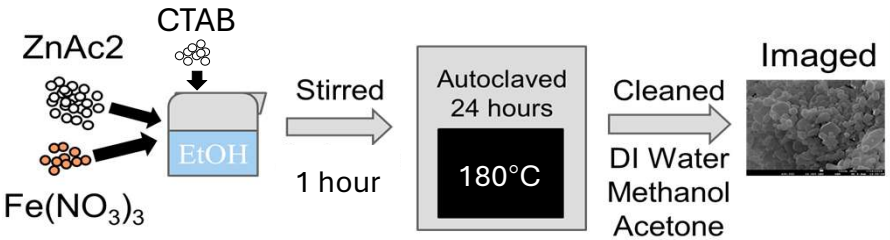
- **Why Fe doping matters:** Adding Fe can **stabilize ZnO surfaces** by reducing internal dipoles and passivating dangling bonds.
- **Bactericidal mechanism focus:** ZnO toxicity may come from **surface defect sites releasing Zn^{2+} ions** during interactions with bacteria or growth media.
  - **Expected Fe effect:** Fe doping should **lower reactive defect-site density**, reducing Zn^{2+} release and altering antibacterial activity.
- **Study goal:** Systematically examine **bulk and surface changes** in hydrothermally synthesized Fe-doped ZnO at different dopant concentrations.

Main objective: Link **Effects of Fe-Doping to Optoelectronic, Structural, and Antibacterial changes in microscale ZnO behavior.**

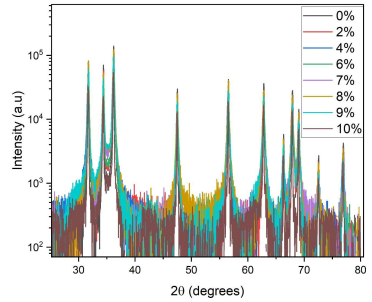
SEM:



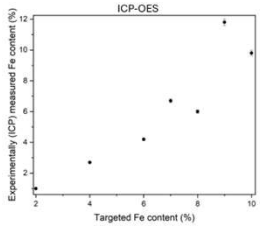
Method:



XRD:

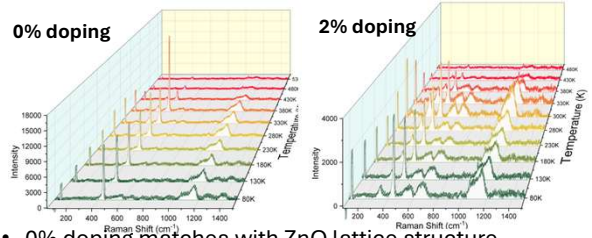


ICP-OES:



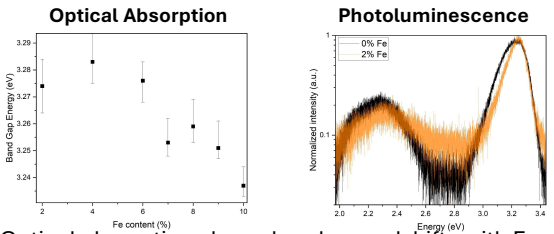
- Shows success of controlled incorporation of Fe into the ZnO lattice.

Raman Spectroscopy:



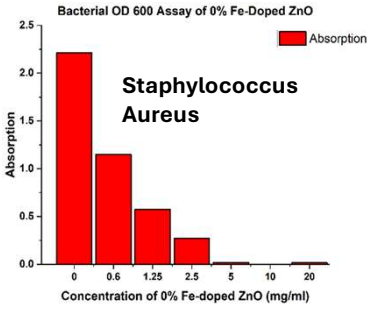
- 0% doping matches with ZnO lattice structure
- 2% doping shows dampening of primary vibrations while maintaining vibrational pathways

Band Gap Manipulation:



- Optical absorption shows bandgap redshifts with Fe
- Photoluminescence shows similar BG/Defect band ratios; suggesting similar optical pathways between both

Antibacterial:



Future Work:

- Generate antibacterial assays with doped samples
- Run higher resolution surface defect analysis

Conclusions:

SEM shows nano-/miroscale material generated. XRD and Raman shows hexagonal wurtzite lattice, matching with ZnO literature. ICP-OES, Raman, and optical absorption has shown successful incorporation of Fe into the lattice. Photoluminescence and optical absorption has shown Fe doping changes optoelectronic properties. Antibacterial activity has been seen with ZnO without doping.