

UTEP – Single Crystal Project Request

Please fill out both sections below and submit by email to: aggoos@utep.edu

Section 1 (form)

<p>Name(s): _____</p> <p>Email: _____</p> <p>Research Group/Affiliation: _____</p> <p>Date: _____</p> <p>Proposed Formula: _____</p> <p>Sensitive to: <input type="checkbox"/> Air <input type="checkbox"/> Water <input type="checkbox"/> Light <input type="checkbox"/> Temperature</p>	<p>For X-ray Facility Use Only: (do not fill this area)</p> <p>Project code: _____</p> <p>a= b= c= α= β= γ= Vol: Å³ Temp: K</p> <p>Symm: _____ Size: _____</p> <p>Date: _____ # Runs: _____</p> <p>Resolution: _____ 2Φ: _____ R(int): _____</p> <p>Total data collection time: _____</p>
<p>Proposed Structure:</p>	<p>Chemical Reaction/Production method: include all solvents used</p>

Section 2 (abstract)

Please provide a short abstract that includes a project description and explains the need for and role of x-ray experiments. Please follow format (see example below).

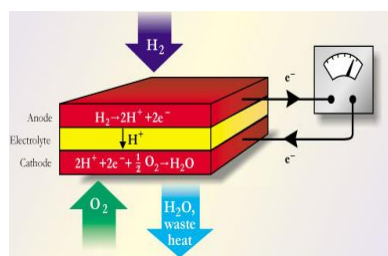
Font: Calibri, **Title:** 18, Bold, centered, **Text:** 14, regular, justified

Should include: 1) PI: 2) Students: 3) Project Description: min 125 words, max 175 words 4) Need for x-ray methods / use of XRSLab:- min 50 words, max 100 words 5) Include a figure related to your project (smaller than 200 x 200 pixels)

In-doped Tin Pyrophosphates as Efficient Intermediate-Temperature Fuel-Cell Electrolytes

PI: Dr. Cristian E. Botez (Physics)

Students: Heber Martinez (MASE Ph.D. Interdisciplinary Program)



Project Description: Novel functional materials that can operate as fuel-cell electrolytes at intermediate temperatures (within the 150°C - 500°C range) are of particular importance for large scale clean-energy applications (e.g. in the automotive industry), as well as for more specific applications based on the

portability and low noise of these devices. Good candidate materials have to exhibit a large proton conductivity at intermediate temperatures, and, among them, In-doped tin pyrophosphates ($In_xSn_{1-x}P_2O_7$) present an interesting case. Their enhanced proton conductivity is not due to a polymorphic structural transition (as for their solid-acid counterparts); similar structures have been reported for all doping levels and operating temperatures. Yet, the $In_{0.1}Sn_{0.9}P_2O_7$ ($x=0.1$) compound has the highest proton conductivity within the series, and understanding the subtle crystallographic modifications that occur when exactly 10% of the Sn atoms are replaced by In is necessary in order to reveal the microscopic details that enhance the proton transport. Eventually, these findings could be used to tune the proton conductivity via chemical manipulation, with the eventual goal of synthesizing more efficient intermediate temperature fuel cell electrolytes.

Need for x-ray methods / use of XRSLab: High-resolution powder diffraction is an ideal tool for the above-mentioned structural studies because of its ability to reveal subtle crystallographic modifications with sub-Ångstrom resolution. In addition, the controlled-sample-environment capabilities afforded by the XRK reactor allows us to investigate the crystal structures (and structure modifications) of the title materials at different temperatures and under different gas atmospheres (flow, pressure).