Hawaiʻi Natural Energy Institute Research Highlights

Advanced Materials

UH & UW Materials Research and Education Consortium (MRE-C)

OBJECTIVE AND SIGNIFICANCE: The objective of the University of Hawaiʻi (UH) and University of Washington (UW) Partnership for Research and Education in Materials (PREM) program is to develop foundational knowledge about advanced nano-to-macroscale defect-bearing and doped materials and the properties controlling their unique behaviors, and investigate their use for future energy technologies. If successful, the project would develop the foundation necessary for increasing participation in materials science and STEM at undergraduate and later graduate level by underrepresented groups (URGs), enabling diverse student participants to perform research at the frontiers of the world's greatest materials research challenges.

BACKGROUND: This project is focused on bringing Materials Science and STEM participation by unique, URGs, in particular Native Hawaiians and Pacific Islanders (NHPI), women and Veterans to equity, by creating a pathway that recruits and retains participants and keeps them on track towards degree attainment. The Seed PREM is configured to capitalize on synergistic expertise and exceptional resources in materials syntheses and characterization available at UH and UW to create close interdisciplinary research collaborations emphasizing the education and training of a diversified next generation of scientists and engineers.

The research on defect-bearing and doped materials is organized into four thrusts aligned with UW's Materials Research Science and Engineering Center Interdisciplinary Research Groups (MRSEC IRGs) on Defects in Nanostructures and Layered Quantum Materials: 1) Dopant control in boron compounds for tailored gas sorption; 2) Defect modeling, characterization, and engineering in ordered vacancy compound chalcopyrites for photovoltaic applications; 3) Role of hydrogen in the chemistry of proton-irradiated solids; 4) Strain control of electronic and magnetic properties of solid materials. The results of this research would lead to new materials and understanding of new phenomena critical for solving emerging needs in energy storage and durable space technologies.

The project creates a pathway to recruit, retain, and ensure degree attainment by over 10 student STEM participants, mostly from the targeted URGs. The research and education initiatives are targeted to encompass: strong student dual-mentoring by both UH and UW senior participants; annual in-person faculty/student summer research exchanges, complimented by regular virtual exchanges; UH-UW co-development of teaching materials; joint seminars; and an annual student symposium.

PROJECT STATUS/RESULTS: The major focus of the past period has been the recruitment and training of PREM undergraduate students into the four research thrusts. The M.O.R.E. strategy encompassing mentoring (M), outreach (O), materials research (R), and materials science education (E) was at the core of implementing MRE-C's objective, including development of a MRE-C website.

The MRE-C research thrusts capitalized on the synergistic expertise of its five UH and seven UW research faculty, and the two institutions' complementary syntheses and characterization resources to create close interdisciplinary collaborations across 7 disciplines which involved training of seven undergraduate students, three graduate students, and three postdocs, inclusive of 4 student exchanges.

Figure 1. UH-UW faculty at a UW-MRSEC Annual All-Hands Workshop, discussing ways to further enhance UH-UW research and education collaborations.

The activities in the four research thrusts were centered on training the student participants, on review of thrust research literature on syntheses and characterization methods, designing and setting up of experiments, performing experiments involving the introducing of defects or dopants into boron compounds, chalcopyrites and mineral oxides, and characterization of materials using XRD and TEM.

Through these efforts the *dopant control in boron compounds for tailored gas sorption* thrust led to the syntheses of nanosized metal borides using mechanochemical and ultra-sonication approaches resulting in discovery of solvents and dopants/additives for metal diborides nanosizing. The current work indicates effective perturbation of bulk TiB_2 structure using alcohol based solvents containing minute amounts of polyethylene glycol.

The *defect modeling, characterization, in ordered vacancy compound chalcopyrites* thrust is in process of developing a manuscript co-authored by UH and UW, on the effect of Al_2O_3 on the photovoltaic performances of chalcopyrite solar materials. This UH-UW collaboration on uncovering the role of Al_2O_3 treatment on defect passivation of chalcopyrites using spectroscopic techniques, is showing PL energy intensity and distribution spectra with a sharp peak at 1.7 eV at low and higher temperatures (4.5K to room temperature) unusual for chalcopyrites with an absorber's bandgap of 1.0 eV.

The thrust on *determination of role of hydrogen in* the chemistry of proton-irradiated solids has effectively prepared proton irradiated mineral oxide samples showing blistering on their surfaces, for further studies using TEM spectroscopy. The oxide samples were polished using focused ion beam (FIB), followed by the irradiation of the samples with D_2^+.

The fourth thrust on *strain control of electronic and magnetic properties of solid materials* synthesized a metal organic ionic salt with potential for spin crossover, $Fe_4(OAc)_{10}[EMIM]_2$ and confirmed the crystal structure using XRD. DFT simulations of the spin crossover behavior of the $Fe_4(OAc)_{10}[EMIM]_2$, suggest spin crossover behavior of the Fe^{2+} at ~49 GPa.

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