

COVER PAGE

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ACCOMPLISHMENTS

A multi-institute partnership between Southern Methodist University (SMU), University of Texas at El Paso (UTEP), and Pacific Northwest National Laboratory (PNNL) has been initiated through this program to address the Department of Energy's Priority Research Opportunities for Carbon-Neutral Hydrogen Technologies. These include (1) discovering and controlling materials and chemical processes for carbon-free production of hydrogen from water; (2) manipulating hydrogen interactions with materials to harness the full potential of hydrogen as a fuel; (3) elucidating the structure, evolution, and chemistry of complex interfaces for energy- and atom-efficiency; and (4) understanding and limiting degradation processes to enhance the durability of hydrogen systems. To this end, we aim to understand hydrogen interactions and dynamics in atomically precise coinage metal-hydride clusters. Because of their well-resolved crystal structures, coinage metal-hydride clusters are attractive candidates for studying structure-property-function relationships in energy sciences with atomic precision. However, determining the hydride locations in their crystal structures is extremely challenging because of the difficulty in growing large and high-quality single crystals for neutron diffraction. This project aims to directly address these knowledge gaps by developing high-precision methods to synthesize and study the structures of coinage metal-hydride clusters by combining different approaches, including spectroscopic, X-ray, and neutron diffraction techniques.

To this end, we have succeeded in synthesizing a series of hydride-containing coinage metal clusters. Examples of such clusters include some with entirely novel compositions (as determined through preliminary spectroscopic analyses) as well as some previously reported silver clusters protected by mixed monolayers of phosphine and hydride ligands. Although the atomic composition of these clusters were determined through mass spectrometry in previous studies, the crystal structures of these clusters are not known. In this regard, one postdoctoral fellow and four undergraduate students in our laboratory are currently optimizing the large scale syntheses and single crystal growth of such hydride-containing silver clusters. Preliminary suggests that phosphine ligands with bulky, rigid functionalities might aid in the growth of high-quality single crystals of these clusters. Work is currently underway to prepare sufficient quantities of cluster samples for X-ray and neutron diffraction analyses.

Additionally, we have made progress towards broadening participation of researchers at all levels at SMU (undergraduate to postdoctoral scholars). Weekly research group meetings are held wherein all researchers present their research results using MS Powerpoint presentations, thereby enhancing their oral communication and presentation skills. In the process, the students are also taught relevant scientific softwares including Mercury, Chem Draw, and Origin. Overall, these efforts are expected to expose students at SMU to multiple different approaches to answer complex research questions, thereby developing essential skills needed for leadership roles in STEM fields.

PRODUCTS

The products shown below include only Publications with a 'Published' status and Intellectual Properties with a 'Granted' status. Products with other statuses are not included in this report. The Revision Type indicates whether a product is New (newly added), Updated (existing product modified), or No Change (existing product reported without modifications) during the current budget period. Note that 'Updated' statuses may appear more frequently as products progress through the publishing process. All products listed have been reported for the current project period of this award.

PUBLICATIONS

There are no publications to report.

INTELLECTUAL PROPERTIES

There are no intellectual properties to report.

PARTICIPANTS AND OTHER COLLABORATING ORGANIZATIONS

The table below only contains participants who have identified an affiliation with the Awardee Institution. Participants from any associated subawards may not be included in this count.

PARTICIPANTS DETAIL

Project Role	Number of People	Total Person Months Worked
Co-Investigator	4	0
Postdoctoral (scholar, fellow or other postdoctoral position)	1	3
Principal Investigator/Project Director	1	1
Undergraduate Student	4	7
Total Responses	10	11

PARTNERS DETAIL

There are no partners to report.

IMPACT

The project has allowed the PI and her students to talk about atomically precise metal cluster hydrides, which have the potential to play a big role in energy sciences in the coming years, to general audiences including REU students from different departments as well as high school students. These efforts are expected to enhance Science communication efforts and make the general public more aware of the critical challenges the world is facing today. Overall, these practices should encourage more students to participate in energy research.