South Dakota NASA EPSCoR FY2023 Major Research Grant (Approved for a three-year project)

South Dakota investigator(s) and	Project title	Funding	NASA and Other Collaborators
affiliation		summary	
• Admin. PI at SDSM&T: Edward F.	Scalable,	\$750,000	 <u>NASA Jet Propulsion Laboratory</u>:
Duke, Director SD NASA EPSCoR	High Energy	(NASA)	Marshall Scott, William West
• <u>Co-I, Science-PI at SDSMT</u> : Weibing	Density		 <u>NASA Glenn Research Center</u>:
Xing	Lithium-	\$375,000	James Wu
• <u>Co-I's at SDSM&T</u> : Tula Paudel ,	Sulfur	(Match)	 <u>Idaho National Laboratory</u>:
Rajesh Shende, Alla Smirnova	Batteries		Boryann Liaw
• <u>Co-I's at USD</u> : Haoran Sun			• Battery Envisions, LLC:
			Zhiqiang Xu

Project Summary

Scalable, High Energy Density Lithium-Sulfur Batteries (SD-LSB)

Rechargeable lithium-ion (Li-ion) batteries offer performance advantages over lead-acid and nickel-cadmium batteries. Liion batteries, however, are approaching an asymptotic limit of specific energy that is unable to meet NASA future space mission needs. The South Dakota School of Mines and Technology and the University of South Dakota propose to research and develop an advanced, beyond Li-ion, lithium-sulfur (Li-S) battery technology through this project titled Scalable, High Energy Density Lithium-Sulfur Batteries (SD-LSB). Together with our partners, including NASA Jet Propulsion Laboratory (JPL) and Glenn Research Center (GRC), we will pursue five objectives:

- 1. Advance battery material science and engineering to render a Li-S battery with high energy density (greater than or equal to 450 Wh/kg), long cycle life (greater than or equal to 500 cycles), safe operation (Li anode protection, nonflammable electrolyte), and wide temperature range (-40 degrees C to +60 degrees C).
- 2. Apply computational approaches, including machine learning, to guide product development and to understand battery performance improvement from a mechanistic standpoint.
- 3. Improve institutional infrastructure and foster collaborations within the state to advance new research on energy storage and increase competitiveness for future federal, state, and private research support.
- 4. Engage researchers from JPL and GRC and industries for follow-on technology transfer and commercialization.
- 5. Support STEM education and training and workforce development with a special emphasis on Native American communities.

Li-S battery technology is identified as a strategic priority for future aerospace missions. However, Li-S batteries face substantial technical challenges including: (1) low practical specific capacity and fast performance decay due to formation, migration, and shuttling of intermediate lithium polysulfides (PSs); (2) poor power capability due to inherently slow electron transfer kinetics of sulfur/sulfide redox chemistry; (3) intrinsically large volume change of the sulfur cathode leading to battery degradation; (4) safety concerns due to dendrite growth of metallic Li anodes; and (5) limited operational temperature range and flammability issues of the electrolytes. These technical hurdles must be overcome before Li-S batteries can be deployed. In a recent work, our team has discovered a new type of PS-trapping material, nanolayer polymer coated high surface area carbons (NPC). We found that when thin films of NPC were coated on sulfur cathodes, the resultant Li-S battery cells demonstrated a discharge specific capacity of ~1,600 mAh/g, approaching the theoretical value. The weight of the nanoscale NPC thin film on sulfur cathodes is negligible rendering a significant performance gain without sacrificing battery specific energy. Our approach is simple, effective, low-cost, and scalable. Leveraging this finding, SD-LSB proposes to further research and develop this novel approach through three technical thrusts: (1) Develop a free-standing, 3D nanostructured, highly conductive, and NPC-enabled PS trapping capable sulfur cathode. This effort will eliminate the dead-weight of the metal substrate, afford high sulfur content, high power capability, and tolerance to large volume change while effectively trapping PSs to inhibit PS dissolution. (2) Develop a fluorinated nonflammable electrolyte to provide robust protection to the Li anode to suppress dendrite growth and improved safety. (3) Integrate battery materials developed in Thrusts (1) and (2) into batteries and characterize Li-S battery performance. Throughout these R&D efforts, we will carry out fundamental, mechanistic studies via multi-physics, multi-scale modeling including density functional theory (DFT). The proposed approach is expected to help meet NASA needs of next-generation battery energy storage for future space missions.