

International Institute for Carbon-Neutral Energy Research



Advanced Energy Materials Thrust Roadmap

2026 March Revision



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- **Molecular, nano, and bulk material development based on new science of surfaces, interfaces, and microstructures for applications involving H₂, H₂O, and CO₂**

Catalytic materials

- Develop bio-inspired molecular systems for fuel and energy generation by biological and synthetic catalysts
- Produce clean fuels and useful materials from ubiquitous chemicals using solar-based energy

Structural materials

- Develop the basic science that enables optimization of the cost, performance, and safety of H₂ technology
- Derive mechanistic insight into the degradation of metals in high-temperature H₂ to enable the safety of evolving hydrogen technologies that operate at elevated temperature
- Relate the basic science underlying deactivation of catalytic surfaces to industrial approaches for the mitigation of hydrogen embrittlement
- Develop next-generation tribo-systems with higher efficiency and durability to conserve energy.

Molecular and Nano- Catalysts

Projects	Objectives	Research Efforts	Researchers
<p>Project 1:</p> <p>Bio-inspired molecular catalysts for fuel and energy generation</p>	<p>Develop bioinspired molecular systems for alternative lower cost and more energy efficient pathways</p>	<ul style="list-style-type: none"> Develop novel biocatalysts and biomimetic catalysts for H₂-activation and CO₂-reduction Develop bio-inspired molecular catalysts for photosynthetic water-splitting 	<p>S. Ogo K-S. Yoon T. Matsumoto T. Yatabe T. Uchida T. Koide</p>
<p>Project 2:</p> <p>Nanomaterials & nanodevices designed for efficient energy & materials conversion</p>	<p>Develop nanocatalysts for efficient oxidation and production of energy materials</p> <p>Develop nanodevices for active utilization of photon energy based on charge separation at the nanointerface</p>	<ul style="list-style-type: none"> Develop selective electrooxidation catalysts Develop efficient reduction catalysts Develop efficient photo reduction catalysts 	<p>M. Yamauchi Y. Takahashi H. Kobayashi M. Donoshita T. Noguchi</p>

Structural materials

Projects	Objectives	Research Efforts	Researchers
Project 3: Predictive Models of H ₂ - Assisted Cracking	<ul style="list-style-type: none"> Develop physics-informed, predictive models of H₂-assisted cracking in structural materials for technologically relevant loading conditions and temperatures Develop predictive models for the mitigation of H₂-assisted cracking through deactivation of catalytic surfaces 	<ul style="list-style-type: none"> Establish comprehensive physical descriptions of H₂-assisted cracking at the proper size scales Establish relevant constitutive relationships for deformation in H₂-exposed materials Integrate physical descriptions and constitutive relationships into predictive model framework 	M. Kubota B. Somerday H. Matsunaga R. Komoda, T. Tsuchiyama R. Kirchheim P. Sofronis A. Nagao
Project 4: Material Development for H ₂ Service	<ul style="list-style-type: none"> Design cost-competitive materials for performance in H₂ service 	<ul style="list-style-type: none"> Develop higher-strength, hydrogen-compatible steels through advanced material processing methods Characterize and improve hydrogen compatibility of welds 	T. Tsuchiyama B. Somerday M. Kubota H. Matsunaga A. Macadre T. Masumura
Project 5: Low friction and wear technology by control of tribo-interfaces	<ul style="list-style-type: none"> Develop physics-based, comprehensive predictive models to design tribological systems with super low friction and wear in order to improve energy efficiency of machinery across technology sectors 	<ul style="list-style-type: none"> Establish comprehensive description of mechanical and tribo-chemical processes and their changes at tribo-interface 	J. Sugimura Y. Sawae H. Tanaka K. Yagi T. Morita T. Yamaguchi