Critical Materials Institute

AN ENERGY INNOVATION HUB

CMI Projects for Year 8

Focus Area 1 – Diversifying Supply

Thrust 1.1 Expanding Sources

1.1.11 Lithium Extraction and Conversion from Brines: Parans Paranthaman

Project Description: Lithium has been identified as one of the near-critical elements and is essential for U.S. energy security. About 2% U.S. production and heavy import reliance despite rapid domestic demand growth for lithium ion batteries for electric vehicles provide impetus for CMI. Team is well poised to address the technology opportunities to increase lithium supply. The main goal is to work with potential industry partners and teams and enable a pre-commercial lithium plant in Salton Sea. Early-stage experiments on sorbent synthesis, structure, and characterization; forward-osmosis membrane to concentrate lithium chloride solution; and solvent extraction for lithium recovery and purification.

1.1.12 Critical Material Recovery from Ores and Lean Sources: Vyacheslav Bryantsev

Project Description: Focus is on developing economical methods of recovery of rare earths (RE) from traditional/nontraditional sources including ores, tailings, and processing streams leading to industry adoption of one or more CMI technologies and to expanded domestic sources of critical materials. Emphasis is on improving the economics of producing concentrates via design of selective collectors, improving state-of-the-art leaching efficiency, RE recovery from leachates, and separation of fine RE-containing solids from viscous liquids. Employed tools include supercomputing, laser spectroscopy, X-ray fluorescence, electron microscopy, and a range of separation equipment such as flotation cells, leaching vessels, cyclones, centrifuges, filters, and extraction contactors.

1.1.13 Recovery of Critical Materials as By-Products: Corby Anderson

Project Description: Three tasks focus on cobalt, gallium, germanium, indium, and tellurium recovery from secondary industrial sources or deposits. There is limited, if any, domestic production of these key critical materials. There are U.S. operations and deposits that can serve as sources of these. National Lab partners are actively engaged along with industry to advance technological research and development leading to a domestic source of these materials.

1.1.14 Biologically-Mediated Recovery of Tellurium from Mine Waste: Yoshiko Fujita

Project Descriptions: To assess the potential for biologically-based approaches to recover tellurium from mine tailings. Biorecovery of Te may present a more economical and environmentally friendly alternative than conventional hydrometallurgy. Oxidative bioleaching is widely accepted for copper recovery, and we hypothesize that a similar approach can be applied for Te leaching. The first year of the project is aimed at establishing that microorganisms can facilitate Te solubilization. If successful, follow-on work would evaluate whether microorganisms can transform the leached Te species into nanoparticulate elemental and/or volatile Te forms, resulting in Te enrichment and facilitating its separation for further refinement.

Thrust 1.2 Transformative Processes

1.2.11 New in-silico Molecular Design Methods for Improved Separations: Marilu Perez

Project Description: To enable, for the first time, the deliberate design of organic ligands with predetermined metal ion selectivity. To achieve this objective, we will develop two connected computational methods, involving machine learning and molecular mechanics that predict absolute log K values for the formation of metal-ligand complexes in aqueous solution to an accuracy of +/- 0.3 log K units. Novel log K predicting software will be implemented within existing HostDesigner code to yield the next generation ligand design software capable of identifying novel ligand compositions with optimal affinity and selectivity for a targeted metal ion species.

1.2.12 Low-Temperature Electrochemical Synthesis of Graphite: Sheng Dai

Project Description: To further investigate a recently developed process for the graphitization of amorphous carbon. Current graphitization technology is a very energy intensive process, requiring temperatures reaching 3000°C and taking up to three weeks for synthesis. Our technology requires a significantly lower temperatures of 800 to 900°C. This is achieved via the cathodic polarization of amorphous carbon in molten salts for only two hours. This technology has the potential to reduce the energy intensity of graphite synthesis significantly. Further, traditionally non-graphitizable hard carbons can be graphitized using this technology, enabling diversification in input feedstock including bio-derived sources of carbon.

1.2.14 Enhanced Separation of Critical Materials: Kevin Lyon

Project Description: Separation of individual rare earth elements (REE) is regarded as the most difficult processing step in the production of high purity rare earth oxides for end-use technology applications due to their inherent chemical similarities. The current state-of-the-art for industrial REE separations utilizes solvent extraction with phosphonic acids, a complex process notorious for its excessive chemical consumption, wastewater effluents, and hundreds of processing steps required to produce individual purified REE. This project seeks to enable domestic REE production by providing economically viable and environmentally sustainable alternatives for REE separations using novel separation technologies that significantly reduce capital and operating costs.

Thrust 1.3 New Uses for Co-Products

1.3.12 Science-Enabling Diverse Value Chain Product from Aluminum-Cerium Alloys: Orlando Rios

Project Descriptions: Targets specific science problems to enable diverse value chain development for Al-Ce alloys, identifying interfacial structure and reaction thermodynamics for better strength at elevated temperature, higher ductility, and lower cost. This project investigates the use of REE precursor compounds as feedstock for direct reduction alloying. This technology can be used for large volume casting technologies like die casting and high-performance applications such as turbochargers, pistons and cylinder heads. If successfully developed, this technology will streamline processing of lanthanide precursor compounds improving economic competitiveness and providing a domestic demand stream through aluminum alloying.

Focus Area 2 – Developing Substitutes

2.1.11 Additive Manufacturing of Polymer Based Bonded Magnets: Parans Paranthaman

Project Description: During sintered rare earth magnet manufacturing, the materials wastage can be up to 48%. Additive manufacturing process offer no tooling requirement and almost no wastage. Fabricate near-net shape high-performance magnets with improved corrosion resistance, mechanical properties and thermal stability of up to 150-200°C, reduce the criticality of Nd, Dy, etc. by minimizing the waste generation associated with magnet manufacturing, and reduce the overall cost. The main goal of this project is to develop gap magnets (with BHmax:15-20 MGOe) based on anisotropic NdFeB magnets. Printed magnets can offer 30% volume reduction and improve motor performance by a factor of two.

2.1.12 High-performance, Critical-element-free Permanent Magnets: Vitalij Pecharsky

Project Description: High performance permanent magnets (HPPMs) are critical enabling components in the next generation renewable energy technologies. Development HPPMs containing only earth-abundant elements, such as Fe and Ni is, therefore, required to ensure sustainability. Meteoritic evidence suggests that nearly equiatomic alloy of Fe and Ni crystallizing in a tetragonal (L10) structure exhibits large anisotropy field and supports (BH)max on the order of 40 MGOe, both are necessary for HPPMs. This project focuses upon novel mechanochemical approaches and non-conventional chemical routes, such as redox and metathesis reactions, to create metastable states that can promote chemical ordering, or directly synthesize nearly equiatomic ordered FeNi alloys.

2.1.13 Finite Element Modelling of Magnetic and Electrochemical Systems: Ikenna Nlebedim

Project Description: To bridge the gap between laboratory experiments and performance of materials in a system. It helps experimental efforts to see past properties measured in laboratories and understand the necessary optimizations for finding the market niche for materials developed, optimized or recycled in the CMI. As needed for a given material, the project incorporates different physics (e.g., magnetic, mechanical, and thermal) and their coupled interactions to determine the suitability of the material for any given application. The feedback from the project to experimental efforts is useful for engaging with potential industrial partners or technology licensees. Technology: Properties of materials developed by CMI will be obtained and modelled to determine system performance in critical applications where the materials are used. System design changes will be developed to take advantage of the material properties to enhance performance and/or reduce the use of critical materials.

2.1.14 Reduced Rare Earth Content High Performance Magnets: Andriy Palasyuk

Project Description: To aims for discovery of new, rare earth poor, ferromagnetic materials. This is a multi-pronged science-based approach of looking for (i) new, undiscovered, rare earth poor, transition metal rich binary, ternary and higher compounds and (ii) looking for new or un-appreciated ferromagnets containing abundant and relatively cheap elements. The benefit of such a discovery would be cheaper and more accessible ferromagnetic materials for energy, electronic and transportation applications. Contributes to the deployment of materials that can substitute for today's rare-earth based magnets.

2.1.15 Heterogeneous Sm-Co and Nd-Fe-B Magnets: Baozhi Cui

Project Description: Rare-earth permanent magnets (REPMs) have excellent magnetic properties and have been widely used in energy conversion and storage, telecommunication, consumer electronics, and sensors. However, REPMs are quite brittle and impossible for applications with high stress and vibration. The brittleness also leads to the magnet production loss up to 30%. This project is to produce REPMs (mainly Sm-Co and Nd-Fe-B sintered magnets) mechanically and magnetically stronger than the commercial products while reducing REPM waste rate to < 10%. The novel magnets will be more powerful, more efficient, and less-weight for energy-related applications while reducing the pressure on critical material supply chain.

2.1.19 Predicting Magnetic Anisotropy: Durga Paudyal

Project Description: Identify, develop and employ novel methods to exploit f-elements for use in various novel rare earth lean magnet materials and d-elements for use in improved rare earth free permanent magnet materials by applying advanced theoretical and computational techniques. The research with rare earth lean materials aims at improving permanent magnet performance beyond the current champion Neo-magnets while research with rare earth free materials aims at improving permanent magnet performance at the gap magnet level. The overarching objective of this project is to provide theoretical support and guidance to various experimental magnet thrust projects to discover and develop high performance magnets.

2.1.20 Application Targeted Magnetic Materials: Jun Cui

Project Descriptions: Bridge CMI's magnet research to manufacturing. Several magnet compositions have been identified via CMI's discovery effort. These magnets use less than half of the Nd in the conventional Nd-Fe-B magnet. Although they are less powerful, but they can be used in many applications less demanding on energy product, thereby reduce Nd supply risk. The project will push CMI's discovery effort one step further, to scale the newly discovered compositions up from the current powder form to sintered bulk magnet. The deliverable will be a set of processes that can be adopted by industry for manufacturing these gap magnets.

2.1.22 SmFeN as a Cost-Effective High Performance Magnet: Vitaliji Pecharsky

Project Descriptions: High-performance permanent magnets (PMs) are important components of high-power density electric motors, generators, and other energy conversion applications. The demand for magnetic materials with reduced critical rare earth content is tremendous. The major goal of this project is to develop thermally stable, sinterable Sm2Fe17N3 powders for manufacturing of fully dense, sintered PMs with properties, comparable to Nd2Fe14B-based analogues. We will reach the stated goal by accomplishing the following objectives: 1) improve the thermal stability of Sm2Fe17N3-based powders by targeted chemical substitutions and 2) develop cost-effective synthesis paradigm that avoids surface oxidation of powders, thus preventing losses of coercivity above 200°C.

2.1.23 Enhancing HDDR Powders: Michael Kesler

Project Descriptions: Develop high performance magnet powders for use in different applications, including bonded magnets, with a focus on understanding of thermomagnetic processing for achieving superior magnetic properties over standard processing routes. While application of high fields can affect reaction rates and pathways by altering thermodynamic barriers or interfacial free energies (for example the Zeeman Effect, which effectively increases reactivity of the processing gases), little systematic work has been done on permanent magnets. Compounds with high magnetocrystalline anisotropy are ideal candidates to explore mechanism by which large magnetic fields can enhance grain alignment, chemical ordering and phase selection to improve remanence and saturation magnetization.

Focus Area 3 – Reuse & Recycling

Thrust 3.1 Energy Storage Systems

3.1.11 Li, Co & PGM Recovery from Li-ion Batteries & E-waste: Tedd Lister

Project Description: To addresses recovery of critical elements from electronic scrap and spent Li ion batteries (LIB). Processes being developed are integrated into flow sheets backed by economic modeling to ensure economic viability. Task 1 seeks to develop chemical extractions chemistry for recovering cobalt as well as valuable transition metals using new and commercial extraction agents. Task 2 develops methods to dissolve cathode metals from LIB, selectively extract lithium and recover graphite. Task 3 targets scrap electronics possessing platinum group elements and rare earth elements. Collectively, these tasks are working with industry to develop solutions to take to the next level.

3.1.12 Li-ion Battery Disassembly, Remanufacturing, and Li & Co Recovery: Tim McIntyre

Project Description: This project provides research, development, and demonstration of novel methods that maximize value recovery from Li-ion battery stacks, modules and cells by reuse, remanufacturing, and materials recovery. The project team will examine the feasibility of promising automation processes for economically recovering critical materials. Separation technologies and conversion techniques, including bioleaching, will be examined and tested in laboratory settings. In terms of reuse, approaches to evaluate existing battery capacity and to restore some capacity for reuse will be studied and tested. Techno-economic and life cycle analyses will be used to characterize the benefits of the most promising approaches under different scenarios.

Thrust 3.2 Co-Production

3.2.11 Ce Gettering of Cu and Fe in Aluminum Alloy Recycling: Ryan Ott

Project Description: This project seeks to improve the energy efficiency and economics of Al recycling by using overly-produced rare earth mining by-products (e.g., Ce). Small additions of Ce to selected Al scrap streams increases the alloy tolerances to impurities and improves the overall corrosion behavior. The Ce additions allows for lower quality scrap streams to be used in the production of high-value alloys. This reduces the need for energy and cost intensive high-purity Al additions. The critical materials benefit is the high value market for the low value by-products that are created during mining critical materials like Nd, Pr, Dy etc. This high value market improves the economics of domestic rare earth mining.

3.2.13 Biomaterials for Critical Material Dissolution, Recovery, and Separation: David Reed

Project Description: Modify bacterial strains using state-of-the-art synthetic biology tools and optimize growth conditions to efficiently utilize agricultural wastes for production of organic acids to optimize leaching of critical elements from a variety of solid end-of-life materials. Furthermore, we develop novel biomaterials through cell encapsulation for recovery and separation of REE via column chromatography.

3.2.14 Switchable Solvent Dewatering from Recovery of Critical Materials: Aaron Wilson

Project Description: Advancing non-evaporative thermal-driven switchable solvent water treatment processes to selectively separate salts/metals (purify and soften water) as well as de-water and dry (solutions, slurries, and solids). Switchable solvent treatments can be used in the production and recycling of critical materials to purify and concentrate critical materials or address waste emerging from the same processes. These are some of the most energy and cost intensive steps in the entire critical material lifecycle. Not only can switchable solvent save energy and reduce cost for these steps, but it can recycle water within the processes increasing the effective supply.

Thrust 3.3 Electric Machines

3.3.12 Low Temperature Electrochemical Processing of Rare Earth Elements: Donna Baek

Project Description: Two low TRL technologies are being investigated for separation of REE mixtures: 1) liquid-metal amalgam between selected REEs and gallium via electrochemical means and 2) electrochemical reduction technology which converts REE metal ions dissolved into an ionic liquid into a solid metallic-state by electrochemical means.

3.3.13 Recovery of Critical Materials from Dilute Electronic Waste Streams: Ikenna Nlebedim

Project Description: Employs environmentally safe and economic approaches to recover critical materials from e-wastes. The project currently focuses on rare earth elements diluted in magnets contained in HDDs but will later be extended to other types of e-wastes e.g., motors, medical devices and other system containing critical materials. When and where applicable, other critical materials (e.g., cobalt), contained in the same e-wastes as rare earth elements, are recovered. Ultimately, the project targets elimination of toxic chemicals, minimizing of negative environmental impact and recovery of materials suitable for supply chain.

3.3.14 Separation and Recovery of Dysprosium and Cobalt from E-Waste: Ramesh Bhave

Project Description: Recovery and separation of dysprosium from rare earth elements recovered from scrap magnets, and cobalt from spent lithium ion batteries will be conducted using a supported membrane solvent extraction (MSX) process. After developing the separation methods, the effect of process conditions such as type of extractant, type of extractant diluent, feed solution concentration, feed/strip pH, extractant composition, and feed/strip residence time will be investigated to achieve high purity (>99%), recovery (>95%), and extraction rates for both dysprosium and cobalt recovery. Furthermore, the long-term stability studies of extractants used in MSX processes will also be carried out for process scale-up.

3.3.15 Low-Temperature Chemical-Mediated Reduction of Rare Earth Elements: Aaron Wilson

Project Description: Investigate a low-temperature method of producing metallic rare earths. This process utilizes strong reducing agents to convert rare earth ions to metallic rare earths. This will take place in low-melting point ionic liquids as a solvent. This will result in a metallization process which will operate at 100°C - 300°C which is lower than the current industrially practiced technology which operated at >1000°C. This technology will potentially result in a domestically produced rare earth metal.

Focus Area 4 – Crosscutting Research

Thrust 4.1 Enabling Science

4.1.11 Advanced Search for High-Performance Materials (AS4HPM): Aurélien Perron

Project Description: Development of new advanced materials using less critical elements by leveraging our world class expertise in modeling and simulation techniques such as computational thermodynamics and ab initio electronic structure calculations. This project has definite technological and economic impacts by enabling the development of new (i) High-performance lightweight alloys with improved mechanical properties using elements that are underused (such as Lanthanum and Cerium); (ii) Materials for power electronics and solid-state lightning applications using less critical elements (Gallium and Indium); (iii) Hard magnets using more transition metals (iron, nickel, etc.) and less critical rare-earth elements.

This project will be tightly coupled with experimental efforts across the different focus areas.

4.1.12 Machine Learning Materials Design: Fei Zhou

Project Description: To design and develop advanced alloy materials through computational modeling and analysis enabled by machine learning (ML) algorithms and tools. In particular, ML tools will be developed and applied to accelerate the optimization of thermomechanical properties of Ce-Al alloys, a break-through technology with important impact on the U.S. supply chain for rare earth. ML models will be trained on large amount of experimental and first-principles data in order to make computational suggestions regarding additional dopants and new compositions for Ce-Al alloys with improved mechanical properties and reduced manufacturing cost.

4.1.13 Accelerated Alloy Development and Rapid Assessment: Ryan Ott

Project Description: To rapidly develop new materials and materials synthesis techniques with a focus on materials that are critical to U.S. energy technologies. This includes developing more cost effective high-performance magnets as well as high-temperature Al alloys that utilize mining by-products. We use 3D printing to rapidly synthesize alloys over large composition ranges combined with advanced characterization techniques to quickly identify desirable structures and/or properties.

4.1.16 Crosscutting Thermodynamic Properties of Critical Materials: Rik Riman

Project Description: Enable science as a support, application-based group with crosscutting efforts within CMI. Our objective is to address processing problems involving a wide spectrum of unit operations and propose solutions whose utility is enhanced by thermodynamic modeling. Any data missing from the thermodynamic model is addressed by examining literature and conducting experiments to measure or estimate this data. Simulation and experimental results are provided to collaborators, the rest of CMI, and the greater scientific community via publications and external presentations. All generated thermochemical data is then collated into an inclusive databank readily accessible to all CMI participants.

Thrust 4.2 Environmental Sustainability

4.2.11 Biogeochemical Impacts of Wastes from Critical Materials Recovery: Yoshiko Fujita

Project Description: This project aims at anticipating some potential environmental risks posed by new technologies/processes developed by CMI projects, in particular effects on the functions of microbial communities that are critical for biological wastewater treatment and for mitigation of environmental pollution impacts in near surface ecosystems. Results from this project will guide CMI projects in FA1, FA2 and FA3 in selection of processing conditions and reagents that will lessen the potential for negative environmental impacts and higher waste treatment and or disposal costs.

Thrust 4.3 Supply Chain and Economic Analysis

4.3.11 Roadmaps for Technology Development: John Collins

Project Description: Guide research toward commercially significant breakthrough and perform market analysis and creates application-specific roadmaps to guide research across several focus areas toward clean energy applications which are benefited through supply diversification, substitution, and recycling.

4.3.12 Impact of Research on Global Material Supply Chains: Ruby Nguyen

Project Description: Provides economic analyses to capture CMI's impacts on the supply chain using various modeling and simulation techniques such as system dynamics, agent-based modeling, deterministic and stochastic optimization, real options and game theory. In addition, high-level and basic material analyses independent from other CMI projects are conducted to evaluate promising feedstock sources and markets.

4.3.13 Optimizing the Economic Performance of CMI Technologies: John Sutherland

Project Description: TEA is a technique that combines production cost modeling with customer/financial analysis to provide decision-making insight to R & D. Our commitments calls for: (1) performing Techno-Economic Assessments (TEAs) in collaboration with CMI researchers at the earliest TRL stage possible; (2) Develop TEA Software Tool for CMI scientists/engineers.

4.3.14 Criticality, Life Cycles, Material Flows and Scenarios: Rod Eggert

Project Description: For all relevant critical and potentially-critical materials, provide (1) forward-looking criticality assessments and underlying economic analysis; (2) life-cycle assessments; and (3) material-flow and scenario analyses.