National Science Foundation PIRE PDC Project and MatCom-ComMat Joint Workshop 2024

Kansas State University Alumni Center, Manhattan, Kansas, USA

June 24-26, 2024

NSF-PIRE Workshop Presenters
Monday, June 24, 2024, 08:30 AM – 04:30 PM

Day 1, June 24, 2024 **Workshop location:** Kansas State University Alumni Association			
Kansas, USA (Central)	**Presenter**	**Affiliation**	**Talk Title (Tentative)**
08:45 AM	Professors Gurpreet Singh, Ralf Riedel, Martin Heilmaier		Welcome remarks/overview
09:00 AM	Prof. Richard Laine *(Keynote)* see appendix for more info)*	University of Michigan	A New Route to High Entropy Nitride Compounds
9:30 AM	Prof. Gunter Motz (Invited)	University of Bayreuth	Ceramic Nonwovens with Exceptional Properties from Silazane/Polyacrylonitrile Hybrid Polymers
10:00 AM	Kai Huang (remote)	University of Padova	Volumetric Additive Manufacturing of SiOC Ceramic by Xolography.
10:30 AM BREAK			
10:45 AM	Doug Hardy	Starfire systems	Brief overview of Starfire Systems
11.00 AM	Prof. Chrystelle Salameh (Invited)	University of Montpellier	From molecular precursors to 3D objects: Advancements in Additive Manufacturing of Ceramics
11:30 AM- 1 PM LUNCH BREAK			
1:00 PM	Arijit Roy	K-State	C60 Infused Silicon Oxycarbide Composite Fiber mat and Performance as Battery Electrode
1:20 PM	Joel Garcia	Lehigh University	Experimental Construction and Structural Investigation of SiC-Cf PDC Composite via Polymer Infiltration Process
1:40 PM	Mitchell Falgoust	U. Texas at Arlington	Machine-Learning Interatomic Potentials for the Simulation of Pyrolysis of Polysiloxanes
2:00 PM	Mohammed Rasheed	K-State, Virginia Tech	Preliminary Data on Preparation and Characterization of Si(X)CN Carbon Fiber Mini-Composite
2.20 PM BREAK			
2:40 PM	Takhya Holly (remote)	U. Texas at Arlington	Kinetic Analysis of a Carbon-rich SiCO Model System

3:00 PM	Hannah Hayes (remote)	U. Texas at Arlington	Pyrolysis Under 'Inert Atmospheres (N_2, Ar, He)' with substantial mass gain — a Hypersensitive SiCO Material
3:20 PM	Narges Malmir	K-State	Direct Ink Writing for Fabricating ZrC Fuel Elements
3:40 PM	Rafid Hussein	K-State	Micro-processing of Zirconia/Graphite Nano Powders using Pico-second Laser Pulses
4:00 PM	Murilo Amaral (remote)	K-State/UNICAMP	Contribution of Ceramic-based Sulfur Hosts for Long-term Cycling Lithium-Sulfur Batteries
4:20 PM-4.30 PM	Paul Owiredu	K-State	Preliminary results on preparation of HfC/SiOC Ceramic Composite Powders
5 PM-6 PM HAPPY HOUR			

MatCom-ComMat Workshop Presenters
Tuesday, June 25, 2024, 1:15 PM– 4:00 PM

Visit to Konza Praire: 08:00 AM to 11:30 AM
Lunch: Noon to 1:15 PM

Day 2, June 25, 2024 **Workshop location:** Kansas State University Alumni Association			
Kansas, USA (Central)	**Presenter**	**Affiliation**	**Talk Title (Tentative)**
1:30 PM	Samuel Kredel	Technische Universität Darmstadt	Thick Ceramic Barrier Coatings Derived from Transition Metal Modified Polyorganosilazanes
1:50 PM	Minoo Boroojerdi (prerecorded)	Technische Universität Darmstadt	Single-source precursor synthesis of ceramic nanocomposites for (ultra)high-temperature applications
2:10 PM	Ingrit Nurak	Karlsruhe Institute of Technology	Microstructural and Chemical Developments at the Interfaces between MoSiTi/Bond Coat/PDC (Polymer Derived Ceramics)
2:30 PM	Büsra Prill	DECHEMA	High temperature oxidation behaviour of ceramic coatings based on PDC-NCs - Improvement of coating properties by oxide filler addition
2:50 PM BREAK			
3:10 PM	Mozhdeh Fathidoost (prerecorded)	Technische Universität Darmstadt	Thermomechanical properties of ceramic-nanocomposite-based monoliths and coatings
3:30 PM	Jurica Filipovic	Technische Universität Darmstadt	Mechanical Characterization and Diffusion Modeling of Aluminide Diffusion Coatings on Molybdenum Substrates
3:50 PM-4:10 PM	Gabriely Falcão	Karlsruhe Institute of Technology	Development of ductile and oxidation resistant Cr-Mo-Si alloys
6:00 PM CONFERENCE DINNER [@Tallgrass Tap House]			

MatCom-ComMat Workshop Presenters
Wednesday, June 26, 2024, 09:30 AM– 11:40 AM

Day 3, June 26, 2024, **Workshop location:** Kansas State University Alumni Association			
Kansas, USA (Central)	**Presenter**	**Affiliation**	**Talk Title (Tentative)**
9:30 AM	Lukas Korell	DECHEMA	Hot corrosion behaviour of Mo-based alloys
9:50 AM	Sri R. Ramdoss	Karlsruhe Institute of Technology	Small scale deformation and failure of Mo silicides
10:10 AM	Arun R. Chitra	Karlsruhe Institute of Technology	Thermodynamic assessment of Cr-Mo-Si system
10:30 AM BREAK			
10:50 AM	Hongmin Zhang	Karlsruhe Institute of Technology	Phase-field simulations of multiphase microstructural evolution in Mo-Si-based ternary alloy
11:10 AM	Hemanth Thota	Karlsruhe Institute of Technology	Creep-induced microstructural evolution of the eutectic Mo-Si-Ti alloy by correlative electron microscopy
11:30 AM	Martin Heilmaier, Ralf Riedel, Gurpreet Singh		Closing Words
11:40 AM LUNCH			

DINING INFORMATION (Location/Hours)

BREAKFAST (7:00 to 8:15 AM): Breakfast will be available on June 24, 25, 26 and 27. It is covered in the registration fee.
Option 1: Kramer Dining Center (1835 Claflin Rd, Manhattan, Kansas 66502) is located 1 km from your hotel. *Please collect meal cards during hotel check-in.*

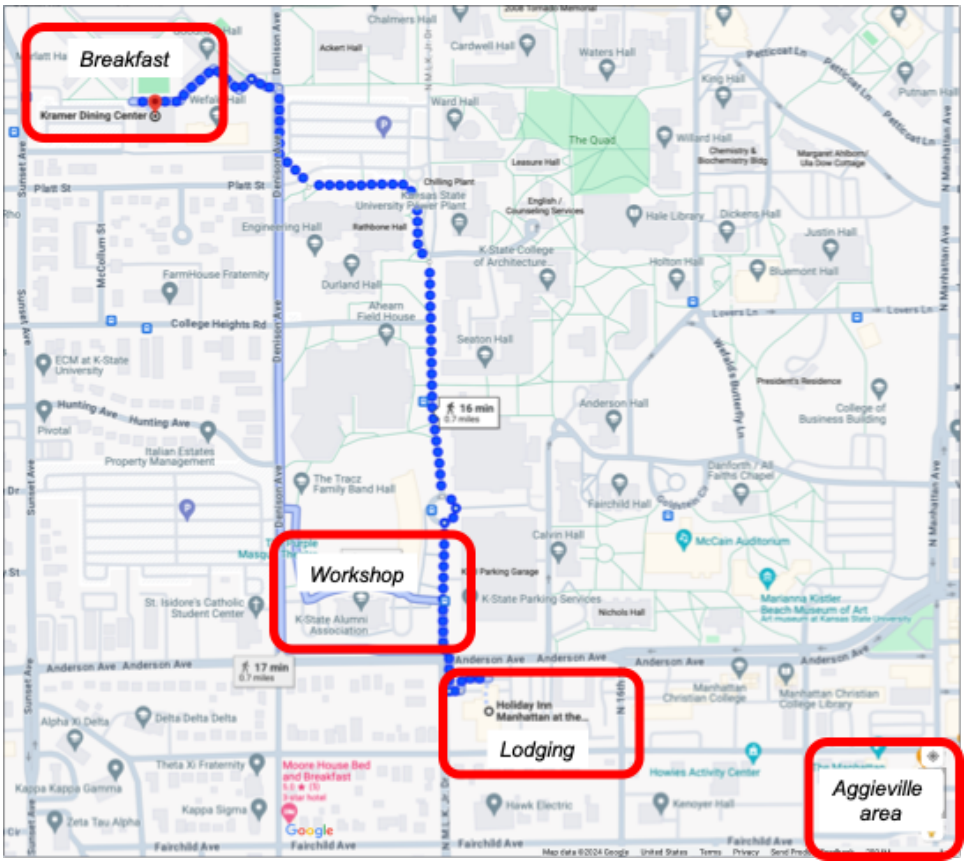
At the front desk of Kramer Dining Center, please present your key card and the person at the counter will swipe your card and allow access to the Dining Center.

Option 2: Other option for breakfast is at your lodging hotel--Holiday Inn Hotel.
You may try either one or both at no additional charge to you. Kramer dining is highly recommended. It is a pleasant walk from hotel to Kramer, you will enjoy it!

LUNCH (approx. 11.30 AM to 1 PM): Catered lunch will be served on June 24, 25 and 26 at the workshop location and is covered in the registration fee.

CONFERENCE DINNER: Conference Dinner on June 25 at 6 PM at the *Tall Grass Tap House* (320 Poyntz Ave, Manhattan, KS 66502) is covered in registration fee. *Alcohol drinks not covered.*

DINNER (other days): Check out restaurants and bars in Aggieville area. It is walkable distance from your hotel. Explore on your own.



IMPORTANT INFORMATION REGARDING VISIT TO KONZA PRAIRIE

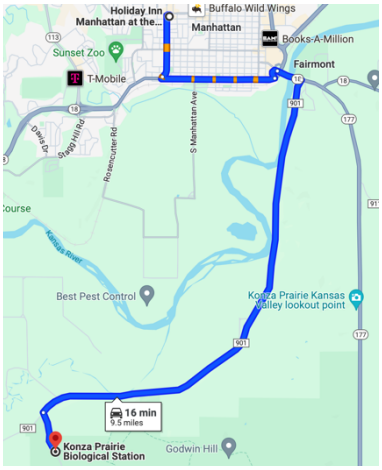
JUNE 25, 2024

Departure: 08:00 AM from Holiday Inn, **Return:** 11.30 AM

Konza Prairie address for car GPS (for those carpooling/rental car): *100 Konza Prairie Ln, Manhattan, KS 66502*

http://keep.konza.k-state.edu/visit/

Hike to the Konza Prairie: If you plan on hiking the Konza Prairie, do bring a pair of hiking boots, sunglasses, hats, bug spray and sunscreen. If the weather is bearable, we may try the 4-mile or 6-mile loops. We plan on leaving from outside of Holiday Inn 08:00 AM.



Kramer Dining Center may offer Breakfast on the go, grab a box of food and you can consume it on the drive to Konza!

Consider bringing along sunscreen, bug repellant, and water. There is a porta potty if anyone needs to use the restroom, but it may not be the most hygienic bathroom stop.

Guidelines: Stay on the trail as it is a protected area. Do not take any souvenirs such as plants etc., as it is a fragile ecosystem. No animals or pets allowed.

Expected weather conditions: Manhattan, KS in June/July is hot! Please bring hats, sunscreen, sunglasses, and anything else you will need for coping with the heat.

TRANSPORTATION OPTIONS

Local Transportation

We will have two SUVs (Mr. Sailesh Menon +1 785 477 0605 WhatsApp and Mr. Arijit Roy +1 785 317 1607 WhatsApp) that are able to accommodate 8 passengers for our drive to **Konza trail** and the **Conference dinner location**. This should be enough for those without the rental car. We assume that majority of the attendees will be renting cars for entire duration of the workshop.

Note: In case you are needing pickup from MHK airport, please inform us at least 3 to 5 days before. For those with flights arriving late at night, it may not be possible for us to receive you at the airport. Please consider making UBER reservation prior to boarding your connecting flight.

APPENDIX—About Professor Richard Laine's Keynote Lecture

Title: A New Route to High Entropy Nitride Compounds

Authors: Richard M. Laine, Zeyu Yi
Affiliation: Dept. of Materials Science and Eng., University of Michigan, Ann Arbor, MI
Contact: talsdad@umich.edu

The Laine group has, over the last decades, formulated ceramic precursor design principles in two reviews,[1,2] that can serve as criteria for the work proposed here. These principles focused originally on silicon non-oxide ceramics but need little modification to be useful here.

Processability. A primary focus must be on the synthesis of processable precursors typically defined as meltable, soluble or malleable which implies introduction of extraneous ligands that prevent early crosslinking while imparting processability. Unfortunately, said ligands must be lost on thermal conversion to the target HEN reducing final ceramic yields.

High ceramic yields (CYs). The competing requirement of high ceramic yields means that minimal amounts of extraneous ligands must be introduced such that their loss will not generate large volumes of gaseous byproducts leading to porous final products and low CYs. For SiC precursors, typical polymer precursor densities are 1-1.2 g/cc. Given that fully dense SiC is 3.2 g/cc, then a 100 % ceramic yield could still result in ΔV of ≈ 70 vol. %. More severe ΔV would be expected for VN (6.8 g/cc) and especially HfN (13.2 g/cc) even with 100 % CYs. In this case, thin films may be accessible but typically < 1 μm^3.

Even a processable polymer containing only H ligands would be expected to undergo tremendous ΔV assuming precursor densities of 2.0 g/cc. Thus, there is a balance between processability, mass loss during ceramization, densification and the potential for realizing the correct crystalline phase.

Phase purity. With HENs, it may be that some impurities such as C or Si will improve ΔS and favor stability. The small number of HENs described primarily in the Russian literature to date offer FCC structures.[4–8] To our knowledge there are no publications on the use of precursors to process HENs; although there is one modest patent on the subject.[9] A further observation is that most of the reported materials are sintered at temperatures of 1800-2200 °C. In principle, precursors may reduce processing temperatures given essentially atomic mixing at the outset reducing diffusion distances but not necessarily temperatures needed to access the correct phase purity. In our precursor approach to HENs, we have reported the need to heat to 1800°C to obtain good crystallization of AlN.[10]

References

(1) R. M. Laine; F. Babonneau. Preceramic Polymer Routes to Silicon Carbide. In *The Chemistry of Organic Silicon Compounds*; J. Wiley & Sons, 1998; Vol. 2, pp 2245–2310.
(2) R. M. Laine; A. Sellinger. Si-Containing Ceramic Precursors. In *The Chemistry of Organic Silicon Compounds*; J. Wiley & Sons: London, 1998; Vol. 2, pp 2245–2310.
(3) Colombo, P.; Paulson, T. E.; Pantano, C. G. Synthesis of Silicon Carbide Thin Films with Polycarbosilane (PCS). *Journal of the American Ceramic Society* **2005**, *80* (9), 2333–2340. https://doi.org/10.1111/j.1151-2916.1997.tb03124.x.
(4) Pogrebnjak, A. D.; Bagdasaryan, A. A.; Yakushchenko, I. V.; Beresnev, V. M. The Structure and Properties of High-Entropy Alloys and Nitride Coatings Based on Them. *Russ. Chem. Rev.* **2014**, *83* (11), 1027–1061. https://doi.org/10.1070/RCR4407.
(5) Dippo, O. F.; Mesgarzadeh, N.; Harrington, T. J.; Schrader, G. D.; Vecchio, K. S. Bulk High-Entropy Nitrides & Carbonitrides. *Sci Rep* **2020**, *10* (1), 21288. https://doi.org/10.1038/s41598-020-78175-8.
(6) Lewin, E. Multi-Component and High-Entropy Nitride Coatings—A Promising Field in Need of a Novel Approach. *Journal of Applied Physics* **2020**, *127* (16), 160901. https://doi.org/10.1063/1.5144154.

(7) Moskovskikh, D.; Vorotilo, S.; Buinevich, V.; Sedegov, A.; Kuskov, K.; Khort, A.; Shuck, C.; Zhukovskyi, M.; Mukasyan, A. Extremely Hard and Tough High Entropy Nitride Ceramics. *Sci Rep* **2020**, *10* (1), 19874. https://doi.org/10.1038/s41598-020-76945-y.
(8) Zhang, P.; Liu, X.; Cai, A.; Du, Q.; Yuan, X.; Wang, H.; Wu, Y.; Jiang, S.; Lu, Z. High-Entropy Carbide-Nitrides with Enhanced Toughness and Sinterability. *Sci. China Mater.* **2021**, *64* (8), 2037–2044. https://doi.org/10.1007/s40843-020-1610-9.
(9) Edward J. A. Pope; Kenneth M. Kratsch. PRECERAMIC POLYMERS TO HAFNIUM CARBIDE AND HAFNIUM NITRIDE CERAMIC FIBERS AND MATRICES. 6,403,750.
(10) Zhang, X.; Yu, M.; Indris, S.; Laine, R. M. Reactions of Metal Chlorides with Hexamethyldisilazane: Novel Precursors to Aluminum Nitride and Beyond. *J Am Ceram Soc.* **2022**, *105* (4), 2474–2488. https://doi.org/10.1111/jace.18271.