TECHNISCHE UNIVERSITÄT DRESDEN

DCMS MATERIALS 4.0 SUMMER SCHOOL

Summer School MATERIALS 4.0

Bridging the Scales

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WELCOME

Innovative materials are one of the key technologies for keeping products and industrial processes economically competitive and ecologically sustainable. Materials innovations enable new technological capabilities and drive major societal advancements but typically require long and costly development cycles. A major challenge for materials development is the interplay of different time and length scales relevant for many advanced materials. Reliable theoretical predictions, their experimental verification and technological implementation are crucial in this context. Complementary efforts and the seamless integration of theory, computation and experiment, will result in a remarkable acceleration of the pace of new materials discovery, design and deployment. To fully take advantage of its potential, this scheme has to rely on cross-innovation and convergence of various scientific fields such as materials science, computer science, physics, chemistry as well as information and data science.

This online summer school targets **Master students**, **Ph.D. students** and (early-stage) **Postdocs** interested in or working on topics related to scale-bridging approaches in materials research.

In order to provide the possibility to participate in the Materials 4.0 summer school 2020 under the global challenge imposed by the COVID-19 pandemic, we have decided to have a completely virtual event this year. Under the topic “Bridging the Scales”, we will offer live-streaming / downloads of lectures, an online poster session, virtual hands-on trainings and "meet the experts" chats.

We thank all speakers for their contribution to our Summer School and Springer Nature for sponsoring the poster awards by providing vouchers.

THE ORGANIZERS OF MATERIALS 4.0

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DCMS MATERIALS 4.0 SUMMER SCHOOL

PROGRAM

	Day 1 16-Aug-21 Monday	Day 2 17-Aug-21 Tuesday	Day 3 18-Aug-21 Wednesday	Day 4 19-Aug-21 Thursday	Day 5 20-Aug-21 Friday
12:30-13:00	**Welcome and opening**				
13:00-13:30	David Srolovitz (University of Hong Kong)	Graeme M. Day (University of Southampton)	Prathik Roy, Murat Öztürk (Springer Nature)	Fabian Welschinger (BOSCH)	Josua Vieten (DLR)
13:30-14:00					
14:00-14:30	Poster Session Break	Poster Session Break	Bohayra Mortazavi (Leibniz Universität Hannover)	Poster Session Break	**Closing session**
14:30-15:00					
15:00-15:30	Nina Gunkelmann (TU Clausthal)	contributed talks I (Z. Wang, T. Olfatbakhsh, K. Wang)	Poster Session Break	contributed talks II (S. Das, D. Bayo, M. Atta)	Wing Kam Liu (Northwestern University)
15:30-16:00					
16:00-16:30			Bohayra Mortazavi (Leibniz Universität Hannover)		
16:30-17:00					
17:00-17:30					
17:30-18:00					
all times are CEST **click here for a time zone converter**					
Zoom Link	Click here to join day 1	Click here to join day 2	Click here to join day 3	Click here to join day 4	Click here to join day 5
Zoom Room #	897 1727 5225	856 2115 5342	845 1177 5176	894 4156 4721	860 8578 6574
Zoom Password	uq*1v9Hd	uq*1v9Hd	uq*1v9Hd	uq*1v9Hd	uq*1v9Hd
Poster Session	https://summerschooldresden.de/poster.html				
Color code	Keynote Presentation	Lecture	Hands On Session / Tutorial	Contributed Talks Poster Session	

Click on a name to navigate to abstract and biography

Keynote Presentations, Lectures and Tutorials	
David Srolovitz	Allotropy in Ultra High Strength Materials
Nina Gunkelmann	Materials across the scales- From atomistic simulations to continuum models
Graeme Day	Building a computational engine for the autonomous discovery of molecular materials
Prathik Roy Murat Öztürk	How to Easily Find (And Use!) Reliable Materials Science Information
Bohayra Mortazavi	First-Principles Multiscale Modeling Enabled by Machine-Learning Interatomic Potentials
Fabian Welschinger	Efficient multiscale methods for viscoelasticity and fatigue of short fiber-reinforced polymers
Josua Vieten	Materials Research as a Service – DLR's spin-off ExoMatter
Wing Kam Liu	Hierarchical Deep Learning Neural Network (HiDeNN)-AI for process design and performance prediction of scientific and engineering systems

Contributed Talks	
Zixuan Wang	Predicting phase change material nucleating agents from a purely geometric data-driven approach
Tina Olfatbakhsh	A Highly Interpretable Materials Informatics Approach for Predicting Microstructure-Property Relationship in Fabric Composites
Kangli Wang	Influence of surface and subsurface Co-Ir alloy on the electronic properties of graphene
Shayeri Das	Study of Metallic Clusters in terms of Density Functional Theory Based Descriptors
Djénabou Bayo	Machine Learning the 2D Percolation Transitions
Atta Muhammad	Thermo-physical properties of graphene reinforced thermoplastics: A Coarse-Grained Modeling Approach.

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Materials Genome Engineering

Monday, Aug 16th 2021 – Friday, Aug 20th 2021

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BOOK OF ABSTRACTS

KEYNOTE PRESENTATIONS, LECTURES AND TUTORIALS

DAVID SROLOVITZ

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Allotropy in Ultra High Strength Materials

Allotropic phase transformations may be driven by the application of stress – this is especially well-known for pressure driven transformations. Recent advances in strengthening materials allow for the application of very large shear stresses as well - opening up vast new regions of stress space. The presence of shear implies that phase transformations depend upon the full stress tensor and crystal/grain orientation. We propose a crystal thermodynamics framework for describing phase transformations in polycrystalline solids and apply it through non-linear elasticity and density functional theory calculations. In particular, we consider bcc→hcp transformations in iron, fcc→hcp transformations in nickel, and hcp→fcc transformations in titanium. The results are quantitatively consistent with a range of experimental observations in these disparate systems.

Biography

David Srolovitz is the author of over 500 research papers on materials theory/simulations of defects, microstructure, deformation, and film growth and has an h-index of 100. He is a Member of the US National Academy of Engineering, Fellow of MRS, TMS, ASM, Institute of Physics and is the winner of the MRS Materials Theory Award. He was a staff member at Exxon Corporate Research and Los Alamos National Laboratory and the Executive Director of the Institute for High Performance Computing in Singapore. He has been a professor at the University of Michigan, Princeton University, Yeshiva University, the University of Pennsylvania, and the City University of Hong Kong. He has held faculty positions in Materials Science, Mechanical Engineering, Aerospace Engineering, Computer Science, Physics, and Applied Mathematics. He is currently Chair Professor of Mechanical Engineering at the University of Hong Kong.

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NINA GUNKELMANN

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Materials across the scales- From atomistic simulations to continuum models

Simulations in material science often require a combination of different methods that act on different length scales. One example is the wear behavior of components. Friction is a phenomenon based on the interaction between macroscopic and microscopic aspects. The combination of molecular dynamics and finite element methods -- sequentially by determining required parameters for the higher scale method or coupled by using MD domains for the boundary of contact bodies modelled in FE -- is a proven approach to solve friction problems.

Another important example is plasticity of metals where multiple phenomena occur at different scales, such as dislocation glide, phase transitions and twinning. It is possible to investigate the elementary mechanisms by using atomistic methods in order to study dislocations or interface structure and mobility. However, the usage of atomistic methods is limited in terms of the accessible computational time and length scales, which prohibits the simulation of complex phenomena involving multiple dislocations and low-symmetry interfaces. Therefore, to account for this complexity, it is necessary to adopt mesoscale approaches, like discrete dislocation dynamics or dislocation density-based continuum theories that describe the dislocation flow through transport equations. In order to predict dislocation behavior, it is, however, necessary to incorporate input based on the lower scales.

This talk will discuss different approaches to the transition from atomistic scale to larger scales. We quantitatively analyze different dislocation microstructure and transfer the information from the nanoscale to the meso and continuum scale. In this way, we are able to provide properties of these microstructures, which cannot directly be captured by molecular dynamics data. The goal is to gain a deeper understanding of the macroscopic mechanical behavior of metals.

Biography

Nina Gunkelmann studied physics at the Technical University of Kaiserslautern as well as at the university in Grenoble, France. After graduating in 2012, she worked for two years as a research assistant at the Chair of Multiscale Simulation at the University of Erlangen-Nuremberg. From 2014, she pursued her PhD at the TU Kaiserslautern, finishing it in 2016. This was followed by a year as a Postdoc at the Chair of Materials Simulation at the University of Erlangen-Nuremberg, before she moved to the Institute of Mechanics and Fluid Dynamics at TU Bergakademie Freiberg in 2017. Since September 2017, she has been working as assistant professor for Computational Material Sciences/Engineering at TU Clausthal. Her research focusses on material simulations of heterogeneous structures on the atomistic and mesoscopic scale.

GRAEME M. DAY

University of Southampton, E-Mail: G.M.Day@soton.ac.uk

Building a computational engine for the autonomous discovery of molecular materials

The talk will describe the vision for the development of a computational framework to guide the discovery of functional crystalline molecular materials. Many properties of interest, such as porosity or charge transport, are strongly influenced by the arrangement of molecules in the solid state. However, the structures of molecular crystals are often determined by a delicate balance of weak, competing interactions. Therefore, small changes in molecular structure can lead to large changes in crystal packing and empirical rules for predicting the arrangement of molecules often fail. Thus, our approach to the computational discovery of materials is built around the core technology of crystal structure prediction (CSP), which has developed into a reliable tool for exploring the likely crystal structures associated to a given molecule. When targeting a given function, we assess the relevant properties for this landscape of potential crystal structures, providing what we call an energy-structure-function (ESF) map [1]. After discussing recent examples of how CSP and ESF maps have been used to guide experimental programmes for materials discovery, I will describe how we have started to integrate CSP with methods for chemical space exploration, using both large-scale computation [2] and population-based evolutionary approaches [3]. This presents several challenges before we can fully automate the exploration of the joint chemical-crystal structure space, including the need to accelerate the CSP methods and to automate the interpretation of ESF maps for identifying the best target molecules for synthesis and characterisation. These are areas where we have made use of supervised and unsupervised machine learning [4,5], which will be described.

[1] Functional materials discovery using energy–structure–function maps, A. Pulido *et al*, *Nature* **2017**, 543, 657.

[2] Large-Scale Computational Screening of Molecular Organic Semiconductors Using Crystal Structure Prediction, J. Yang *et al*, *Chem. Mater.* 2018, 30, 4361.

[3] Evolutionary chemical space exploration for functional materials: computational organic semiconductor discovery, C. Y. Cheng, J. E. Campbell and G. M. Day, *Chem. Sci.* **2020**, 11, 4922-4933.

[4] Machine learning for the structure–energy–property landscapes of molecular crystals, F. Musil, S. De, J. Yang, J. E. Campbell, G. M. Day and M Ceriotti, *Chem. Sci.* **2018**, 9, 1289-1300.

[5] Machine-Learned Fragment-Based Energies for Crystal Structure Prediction, D. McDonagh, C.-K. Skylaris and G. M. Day, *J. Chem. Theory Comput.* **2019**, 15, 2743–2758; Multi-fidelity Statistical Machine Learning for Molecular Crystal Structure Prediction, O. Egorova, R. Hafizi, D. C. Woods and G. M. Day, ChemRxiv preprint **2020**, https://doi.org/10.26434/chemrxiv.12407831.v1.

Biography

Graeme Day is Professor of Chemical Modelling at the University of Southampton. His research concerns the development of computational methods for modelling the organic molecular solid state. A key focus of this work is the prediction of crystal structures from first principles; his research group applies these methods in a range of applications, including pharmaceutical solid form screening, NMR crystallography and computer-guided discovery of functional materials. After an undergraduate in Canada (Saint Mary's University), he obtained an MSc in Theoretical Chemistry at Oxford University and a PhD in computational chemistry at University College London. He spent 10 years at the University of Cambridge, where he held a Royal Society University Research Fellowship working mainly on modelling pharmaceutical materials and computational interpretation of terahertz spectroscopy. He moved to the University of Southampton in 2012. Graeme has served on the editorial boards of CrystEngComm, Faraday Discussions, the advisory board of Molecular Systems Design & Engineering (MSDE) and as an Associate Editor for Chemical Science.

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PRATHIK ROY, MURAT ÖZTÜRK

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How to Easily Find (And Use!) Reliable Materials Science Information

The exponential growth of data in the field of materials science has led to vast amounts of information and data being scattered across journals, books and patents making the discoverability of this information difficult. The webinar will illustrate how SpringerMaterials can help researchers and students to identify materials and their properties via use case scenarios. https://materials.springer.com is home to the largest collection of critically evaluated data in materials science and related fields.

Prathik Roy is Group Product Manager at Springer Nature, where Murat Öztürk works as a solution specialist.

We thank Springer Nature for providing the poster awards.

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BOHAYRA MORTAZAVI

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First-Principles Multiscale Modeling Enabled by Machine-Learning Interatomic Potentials

Density functional theory calculations are robust tools to explore the mechanical properties of pristine structures at their ground state but become exceedingly expensive for large systems at finite temperatures. Classical molecular dynamics (CMD) simulations offer the possibility to study larger systems at elevated temperatures, but they require accurate interatomic potentials. Herein the authors propose the concept of first-principles multiscale modeling of mechanical properties, where ab initio level of accuracy is hierarchically bridged to explore the mechanical/failure response of macroscopic systems. It is demonstrated that machine-learning interatomic potentials (MLIPs) fitted to ab initio datasets play a pivotal role in achieving this goal. Our study highlights that MLIPs were the missing block for conducting first-principles multiscale modeling, and their employment empowers a straightforward route to bridge ab initio level accuracy and flexibility to explore the mechanical/failure response of nanostructures at continuum scale.

Biography

Bohayra is a postdoctoral fellow at Leibniz Universität Hannover, Germany. His research area is related to multiscale modeling, materials and systems for energy storage/conversion and machine learning. Prior to joining Leibniz Universität he accomplished 6 years of postdoctoral research in Bauhaus-Universität Weimar and Technische Universität Dresden, respectively. He has held a PhD since 2013 from University of Strasbourg in collaboration with Luxembourg Institute of Science and Technology on the multiscale modeling of thermal and mechanical properties of nanostructured materials and polymer nanocomposites. His Bachelor and MSc studies are related to mechanical/manufacturing engineering, graduated in 2005 and 2008, respectively.

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Efficient multiscale methods for viscoelasticity and fatigue of short fiber-reinforced polymers

In order to predict the nonlinear mechanical behavior of components made of short fiber-reinforced plastics (SFRP) under long term and cyclic loading, seamless methods ranging from the process to the component simulation are required. The injection molding process leads to locally varying fiber orientations within the component. This varying microstructure [1] significantly influences the viscoelastic and fatigue behavior of the component. The scale transition from the microstructure [2] to the nonlinear macroscopic properties is resolved by a coupled FFT-FEM two-scale method, where the fiber orientation tensor is obtained by analyzing µCT images or by process simulations. The aim of this work is to reduce the numerical effort of such a multiscale method. In a first step, the highly efficient micro-scale solver FeelMath [3] for regular grids using a FFT-based pre-conditioner is presented. Afterwards, a numerical scheme based on a precomputed database trained with FeelMath simulations on the microscale and a model order reduction algorithm [4], is discussed. This approach significantly reduces the numerical effort, such that the method is applicable for industrial problems. Comparative studies of the fully coupled and reduced model document the high accuracy of this approach. The overall performance of this methodology is demonstrated by three dimensional, industrial applications.

Biography

2000 – 2005: Studies in Civil Engineering, University of Stuttgart, graduation as Dipl.-Ing.

2005 – 2011: Research Assistant, University of Stuttgart, Institute of Applied Mechanics (Prof. Christian Miehe), graduation as Dr.-Ing.

2011 – 2019: Research Engineer, Robert Bosch GmbH, Corporate Sector Research and Advance Engineering, Plastics Engineering

Since 2019: Senior Expert for Computational Multiscale and Fracture Mechanics, Robert Bosch GmbH, Corporate Sector Research and Advance Engineering, Applied Material and Manufacturing Technologies for Metals and Polymers

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JOSUA VIETEN

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Materials Research as a Service – DLR's spin-off ExoMatter

Materials are an essential part of our everyday lives. The development of high-performance, sustainable and economical materials is the task of R&D departments across different industries. Nowadays, computer-aided methods for materials development are available, but many companies are neither aware of nor use them due to a lack of specialist expertise. Despite the promising possibilities, the level of digitalization in materials development is still low in many industries. We would like to change that.

By using existing repositories of first-principles data, experimental data, and machine-learned materials properties, we aim to create custom databases addressing real business needs. We filter these databases and rank materials according to properties relevant to each individual project. As a holistic R&D service provider and consultant in the B2B sector, we will not only meet the technical and economic requirements of our customers, but also keep the environmental compatibility and sustainability of material production in focus.

ExoMatter is a planned spin-off company of the German Aerospace Center (DLR) with support by the Helmholtz Association. The future founders Josua Vieten and Friedemann Call are currently testing their services with pilot customers such as Carbyon, before ExoMatter will be launched as an independent company in 2022.

The talk will address the rationale behind ExoMatter, show examples of databases and dashboards we create, and explain the process of commercializing research in the form of a spin-off company at a German research institution.

More information about ExoMatter can be found at https://exomatter.ai.

Biography

Josua Vieten is currently managing the spin-off project ExoMatter at German Aerospace Center (DLR). Previous stations include a position as an R&D Coordinator for the quickly-growing software company Celonis and a position as a project manager at DLR. Josua completed his PhD on materials development for solar energy conversion at TU Dresden and DLR in 2019, during which he spent some time in the US at Lawrence Berkeley National Lab. He previously studied Chemistry and Materials Science at TU Munich. Josua is full of ideas and loves turning them into a reality.

WING KAM LIU

Ye Lu, Sourav Saha, Satyajit Majumdar, Abdullah Al Amin, Zhengtao Gan, Xiaoyu Xie, Hui Lin, Jian Cao
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Hierarchical Deep Learning Neural Network (HiDeNN)-AI for process design and performance prediction of scientific and engineering systems

We propose a mechanistic Artificial Intelligence (AI) framework, called Hierarchical Deep Learning Neural Networks or HiDeNN-AI [1, 2] for discovering the mathematical and scientific principle behind engineering systems. The HiDeNN-AI discovery has three sequentially executed steps: (1) using available small amount of data to characterize an unknown physical process through simple mechanistic equation, (2) enriching the database with the mechanistic equation from (1) and training with combined data from the equation and available data to create a reduced order model with uncertainty, and (3) using the reduced order model to generate sufficient data to discover new robust mathematical and scientific principles that are able to (a) perform predictive solutions for design and optimization, and (b) provide simple relationship for online monitoring and control. We have applied this HiDeNN-AI framework to address the Air Force Research Lab (AFRL) AM modeling challenges [3, 4, 5]; and for the prediction of the as-built mechanical properties [6]. To further enhance HiDeNN-AI, a reduced-order modeling method accounting input uncertainty, called the eXtended Tensor Decomposition (XTD) [7], is being developed. The so-called HiDeNN-AI-XTD is expected to solve the general scientific and engineering problems in high dimensional space-time-parametric domains at deep discount in computational cost. Once the offline database is set up, the mechanistic machine learning module of HiDeNN-AI can be activated for process design, real time system monitoring and control or the identification of key processing parameters for the desired performance of the manufactured material systems with uncertainty quantification. Various results comparing the HiDeNN-AI-XTD approach with the conventional machine learning models will be shown using real-time IR in-situ measurement, and high-frequency thermal signatures for the predictions of mechanical properties and the detection of lack of fusion and keyhole porosities.

References

[1] Zhang, L., Cheng, L., Li, H., Gao, J., Yu, C., Domel, R., Yang, Y., Tang, S. and Liu, W.K., 2021. Hierarchical deep-learning neural networks: finite elements and beyond. *Computational Mechanics*, *67*(1), pp.207-230.

[2] Saha, S., Gan, Z., Cheng, L., Gao, J., Kafka, O.L., Xie, X., Li, H., Tajdari, M., Kim, H.A. and Liu, W.K., 2021. Hierarchical Deep Learning Neural Network (HiDeNN): An artificial intelligence (AI) framework for computational science and engineering. *Computer Methods in Applied Mechanics and Engineering*, *373*, p.113452. https://doi.org/10.1016/j.cma.2020.113452.

[3] Gan, Z., Jones, K.K., Lu, Y., and Liu, W.K., 2021, Benchmark study of melted track geometries in laser powder bed fusion of Inconel 625, *Integrating Materials and Manufacturing Innovation* (Accepted).

[4] Saha, S., Kafka, O.L., Lu, Y., Liu, W. K., 2021, Microscale Structure to Property Prediction for Additively Manufactured IN625 through Advanced Material Model Parameter Identification, *Integrating Materials and Manufacturing Innovation,* https://doi.org/10.1007/s40192-021-00208-5

[5] Saha, S., Kafka, O.L., Lu, Y., Liu, W. K., 2021, Macroscale Property Prediction for Additively Manufactured IN625 from Microstructure through Advanced Homogenization, *Integrating Materials and Manufacturing Innovation* (Under review).

[6] Xie, X., Bennett, J., Saha, S., Lu, Y., Cao, J., Liu, W. K., Gan, Z., 2021, Mechanistic data-driven prediction of as-built mechanical properties in metal additive manufacturing, *npj Computational Materials* (Accepted).

[7] Lu, Y., Mojumder, S., Saha, S., Liu, W. K., An extended tensor decomposition model reduction method: training, prediction, and design under uncertainty, *In prep.*

[8] Lin, H., Mao, Y., Carter, F., Gao, Z., Agrawal, A., Liu, W.K., Cao, J. Mechanistic artificial intelligence for defect detection using in-situ IR measurements and physics-informed models, *In prep.*

Biography

Professor Wing Kam Liu is the Walter P. Murphy Professor of Northwestern University, Director of Global Center on Advanced Material Systems and Simulation, Past President (2018-present) and President (2014-2018) of the International Association for Computational Mechanics (IACM), Past Chair (2017-2018) and Chair (2015-2016) of the US National Committee on TAM and Member of Board of International Scientific Organizations, both within the US National Academies. Selected synergistic activities includes the development of ICME multiscale and data-driven theories, methods, hierarchical deep learning neural networks, and software with experimental validations for the design and analysis of engineering material systems, materials design, advanced and additive manufacturing; and technology transfer.

Professor Liu has received numerous major awards and honors including: the 2014 as a highly cited researcher in Computer Science and a member of the World's Most Influential Scientific Minds by Thompson Reuters; the 2013 Japan Society for Computational Engineering and Science Grand Prize in recognition of his outstanding contributions in the field of computational mechanics (bestowed in 2014); the Honorary Professorship from Dalian University of Technology in 2013; the 2012 Gauss-Newton Medal (IACM Congress Medal); the highest award given by IACM; the 2012 ASME Design Automation Conference Best Paper Award; the 2009 ASME Dedicated Service Award; the 2007 ASME Robert Henry Thurston Lecture Award; the 2007 USACM John von Neumann Medal; the 2004 Japan Society of Mechanical Engineers (JSME) Computational Mechanics Award; the 2002 International Association for Computational Mechanics (IACM) Computational Mechanics Award; the 2001 USACM Computational Structural Mechanics Award; the 1995 ASME Gustus L. Larson Memorial Award, the 1985 ASME Pi Tau Sigma Gold Medal; the 1979 ASME Melville Medal (for best paper); the 1989 Thomas J. Jaeger Prize of the International Association for Structural Mechanics, and the 1983 Ralph R. Teetor Educational Award from the American Society of Automotive Engineers.

Liu is an elected life fellow of ASME and ASCE, fellow of AAM, USACM and IACM. He obtained his M.S in 1977 and PhD in 1981, both from California Institute of Technology. In 1976, He obtained by B.S with the highest honor from the University of Illinois at Chicago Circle. He is a Registered Professional Engineer for the State of Illinois. He has over 40 years of engineering and manufacturing consulting, including a broad array of companies and industries, small businesses, and international corporations.

CONTRIBUTED TALKS

52 ZIXUAN WANG

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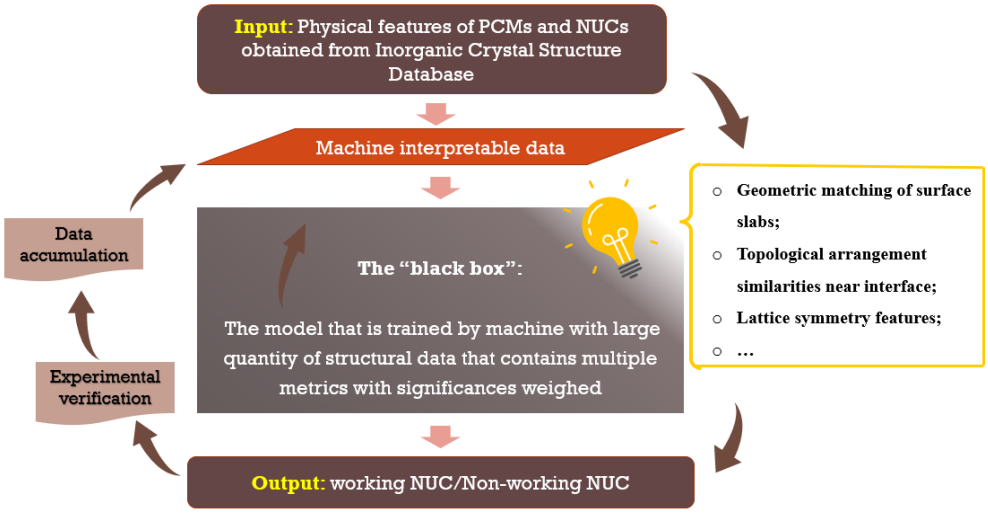
Predicting phase change material nucleating agents from a purely geometric data-driven approach

The latent heat storage/release capacity exhibited by phase change materials (PCMs) offer application for heat storage batteries, provided crystallisation can be controlled through the addition of chemical nucleating agents. Finding suitable nucleators to induce crystallisation at a particular temperature is therefore a crucial but challenging problem. Currently, experimentalists approach the task by systematically testing the stock of chemicals on the laboratory shelf, leading to a huge waste of time, resource, and lack of overall understanding. Using high-throughput data-driven fast screening approach, however, it should be possible to unveil the black box that correlates the common features of both PCMs and nucleators with a binary decision of "working/non-working nucleator". Having access to reliable working (and non-working) PCM/nucleator pair data is critical to achieving a trained model, and to this end this project involves working closely with experimentalists. Using a small pond of known working/non-working pairings, work began with validating a series of metrics, such as geometric, structural and energetic, to rank the likely success of the experimentally-studied PCM/nucleator pairings. In this way, we correctly predicted 17 compounds (from a total list of 18) as working/non-working nucleators for the PCM sodium acetate trihydrate. This success rate, of 94%, was achieved through consideration of geometric matching alone. This process is very fast and has huge potential to find other currently unknown nucleators through mining e.g. the inorganic chemistry structural database (ICSD). This initial training process allowed us to tune parameters and models to build towards devising a workflow that will be a fully automated machine learning process, free from the biases introduced by manually setting the selection criteria. This machine learning approach has huge potential to gain new insights on the processes that drive heterogeneous nucleation, and thus to improve the current efficiencies of heat storage batteries.



32 TINA OLFATBAKHSH

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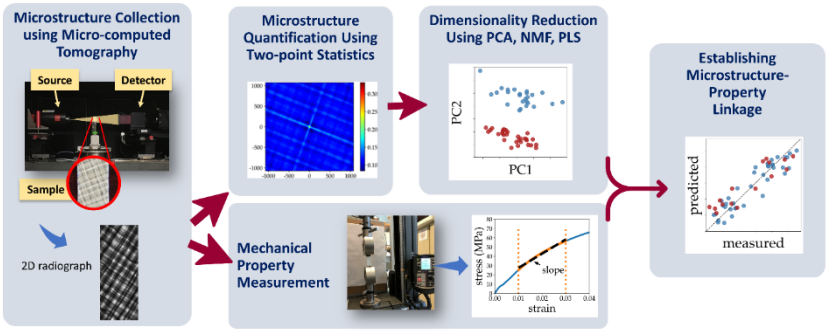
A Highly Interpretable Materials Informatics Approach for Predicting Microstructure-Property Relationship in Fabric Composites

Multi-scale properties of fabric-reinforced composites are commonly modelled via numerical and experimental methods, which are often highly time-consuming and complex [1]. In this research, a materials informatics-based approach has been developed to link the micro/meso-level features of woven fabric composites, obtained via non-destructive micro-CT images, to their effective Young's moduli. To this end, a reduced-order quantification of a typical glass fiber/polypropylene lamina's microstructure is established using two-point spatial correlations and model selection algorithms [2]. Three dimensionality reduction algorithms Principal Component Analysis (PCA), Non-negative Matrix Factorization (NMF) and Partial Least Squares (PLS), are compared in terms of interpretability and competency. Next, a machine-learning model is implemented to predict the material microstructure-property (modulus) relationship via the captured images. Multiple Linear Regressions and Random Forests Regressions are compared and the effect of the manufacturing group on the mechanical property of the final product is investigated using the concept of mixed-effect models. Despite the limited number of samples, the presented data-driven techniques led to a model with highly interpretable components and excellent accuracy for different ply orientations, despite apparent uncertainties such as waviness. The findings appear to be a promising step forward for the potential use of materials informatics for smart design and optimization of woven fabric composites in prominent industries including aerospace and transportation.



References:

[1] K. Rajan, Materials informatics, Mater. Today. 8 (2005) 38–45. https://doi.org/10.1016/S1369-7021(05)71123-8

[2] A. Gupta, A. Cecen, S. Goyal, A.K. Singh, S.R. Kalidindi, Structure-property linkages using a data science approach: Application to a non-metallic inclusion/steel composite system, Acta Mater. 91 (2015) 239–254. https://doi.org/10.1016/j.actamat.2015.02.045.

51 KANGLI WANG

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Influence of surface and subsurface Co-Ir alloy on the electronic properties of graphene

By performing the state-of-the-art first principles calculations, we explore how different compositions of surface and subsurface Co-Ir alloy influence the moir\'e structure, graphene-metal charge transfer, band structure, and stability of a graphene layer on Ir(111), and further compare them with the experimental results. The deeper insights into the interplay between graphene structure and different kinds of Co-Ir alloy from this study are expected to provide a useful guide for achieving precise layer controlled graphene growth and the design of graphene-based devices.

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Study of Metallic Clusters in terms of Density Functional Theory Based Descriptors

Study of metallic clusters has attracted a lot of attention in recent years due to its wide range of applications in optoelectronic, photovoltaics and non-linear optical devices. There are a number of studies reported on bimetallic clusters, however study of trimetalic clusters and its applications is very limited. Among several clusters, system consist of noble metals- Cu, Ag and Au is of high importance due to its interesting electronic and optical properties. In this work, we have investigated structure, electronic and optical properties of Cu_nAgAu (n=1-4) by using Density Functional Theory (DFT) methodology. DFT based descriptors – Highest Occupied Molecular Orbital (HOMO)- Lowest Unoccupied Molecular Orbital (LUMO), molecular hardness, softness, electronegativity, electrophilicity index and dipole moment of these clusters are computed. The computed HOMO-LUMO energy gap are found in the range of 0.711 eV to 1.786 eV. An interesting relationship is observed between HOMO-LUMO energy gap and DFT based descriptors. The HOMO-LUMO energy gap exhibits fascinating odd-even alternation behaviour as a function of cluster size.

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Machine Learning the 2D Percolation Transitions

The percolation model is one of the simplest models in statistical physics displaying a phase transition [1]. A classical lattice is occupied randomly with a given probability at each site (or bond). A phase transition from a non-percolating to a percolating state appears around a probability pc, the so-called percolation threshold. Machine Learning (ML) and Deep Learning (DL) techniques are still relatively new methods when applied to physics. Recent work shows that ML/DL techniques allow to detect phase transitions directly from images of computed quantum states [2,3]. Here, we implement ML/DL techniques to identify the percolation threshold in 2D by identifying the connectivity proper-ties of percolation clusters. We employ a standard image classification strategy with a multi-layered convolutional neural network. In addition, we also work directly with the numerical raw data. The implementation is carried out in Python with the ML/DL libraries of Pytorch [4]. We pay special attention to the question of whether these DL methods can indeed identify percolation, i.e. spanning clusters, or are just counting occupation densities.

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Thermo-physical properties of graphene reinforced thermoplastics: A Coarse-Grained Modeling Approach.

Graphene, being one of the most promising material, has gained attention in scientific and industrial fields. With its superior properties, if introduced in the polymeric matrix can potentially improve material characteristics (such as thermal, elastic, electrical properties, etc). Thus, in this study coarse-grained molecular dynamic (CG MD) simulations were performed to investigate thermo-physical properties such as density, glass transition temperature, coefficient of thermal expansion, Young modulus, Poisson's ratio and thermal conductivity of graphene reinforced thermoplastics (Polypropylene/graphene (PP/Gr) and Polylactic acid/graphene (PLA/Gr) composites).

Initially, we analyzed the thermo-physical properties of neat polymers (PP, PLA) and filler (Gr) using the MARTINI force field [1-2] and compared the results with experiments. Further, CG MD simulations were performed to determine the effect of graphene reinforcement on mechanical as well as thermal properties of PP/Gr and PLA/Gr composites. CG MD simulations show that Young modulus increases with increasing graphene concentration in the PP matrix, and in good agreement with experiments. Graphene reinforcement with wt. = 2% increases the elastic modulus by 35% compared to neat PP. Similarly, enhancement of 12% in elastic modulus has been observed for PLA/Gr composite with similar reinforcements.

We also performed the Non-Equilibrium Molecular Dynamic (NEMD) simulation to quantify the effect of graphene inclusion on the thermal properties of the composite using the Müller-Plathe algorithm [3]. In the case of the PP/Gr composite, effect of graphene concentration on thermal conductivity is negligible; whereas, a slight increase in thermal conductivity was observed in the case of PLA/Gr composite. The thermal behavior of composite is in agreement with literature values, which also show that the graphene concentration less than 5% wt. has negligible effects on the thermal properties of the composite [4]

References:

[1] E. Panizon, et al., J. Phys. Chem. B, 119 (2015), 8209-8216.

[2] X. Li, et al., Acta Mechanica Solida Sinica, 30 (2017), 557-682.

[3] F. Müller-Plathe, J Chem Phys, 106 (1997), 6082.

[4] R. Guo, et al., Polymers, 11 (2019), 549-568.