At-a-Glance Schedule



Conference on **Sian 2024** Mathematical Aspects of Materials Science

May 19-23, 2024 Sheraton Pittsburgh Hotel at Station Square Pittsburgh, Pennsylvania, U.S.

Online Program and Mobile App

Attendees are encouraged to visit

https://www.siam.org/conferences/cm/program/program-and-abstracts/ms24-program-abstracts to view the Online Program Schedule.

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Saturday, May 18

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4:00 p.m. – 6:00 p.m. Registration *Grand Station Ballroom 3 Foyer*

Sunday, May 19

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7:00 a.m. – 5:30 p.m. Registration *Grand Station Ballroom 3 Foyer*

7:45 a.m. – 8:00 a.m. Opening Remarks Grand Station Ballroom 1-2

8:00 a.m. – 8:45 a.m.

IP1 Thin Film Fluid Dynamics Problems with Applications in Materials Science Linda Cummings, New Jersey Institute of Technology, U.S. *Grand Station Ballroom 1-2*

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8:45 a.m. – 9:15 a.m. Coffee Break *Grand Station Ballroom 3-5*

9:15 a.m. – 11:15 a.m. Concurrent Sessions

MS1 Advances in Mathematical and Numerical Techniques for Electronic Structure Calculations -Part I of III Grand Station Ballroom 1-2 MS2 Mechanics and Physics of Growth in Soft and Hard Materials - Part I of III Haselton 1 & 2 MS3 Emergent Properties in Metamaterials and Extreme Wave-phenomena: Analysis, Design, Modeling - Part I of III Woodlawn 1 MS4 Defects in Complex Materials: Interplay between Theory and Computation - Part I of III Pointsview MS5 Transforming Materials and Structures - Part I of IV Ellwood 1 MS6 Machine-learning-enabled Materials' Design -Part I of III Edenburg MS7 Theoretical and Applied Aspects of Nonlocal Models - Part I of III Stoops Ferry MS8 Advances in Probabilistic Methods for Uncertainty Quantification of Complex Systems -Part I of III Brighton 1 MS9 Advances in Variational Methods and Applications to Materials - Part I of III Brighton 2

Sunday, May 19

MS10 Optimal Transport: Theory and Applications Brighton 3
MS11 Interaction of Solid Mechanics and Mathematics: Modelling, Analysis and Applications - Part I of II Brighton 4

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11:15 a.m. – 12:45 p.m. Lunch Break

12:45 p.m. – 1:30 p.m. PD1 Funding Opportunities in the Division of Mathematical Sciences *Grand Station Ballroom 1-2*

1:30 p.m. – 1:45 p.m. Intermission

1:45 p.m. – 3:45 p.m. Concurrent Sessions

MS12 Advances in Mathematical and Numerical Techniques for Electronic Structure Calculations -Part II of III Grand Station Ballroom 1-2 MS13 Mechanics and Physics of Growth in Soft and Hard Materials - Part II of III Haselton 1 & 2 MS14 Emergent Properties in Metamaterials and Extreme Wave-phenomena: Analysis, Design, Modeling - Part II of III Woodlawn 1 MS15 Defects in Complex Materials: Interplay between Theory and Computation - Part II of III Pointsview MS16 Transforming Materials and Structures - Part II of IV Ellwood 1 MS17 Machine-learning-enabled Materials' Design - Part II of III Edenburg MS18 Theoretical and Applied Aspects of Nonlocal Models - Part II of III Stoops Ferry MS19 Advances in Probabilistic Methods for Uncertainty Quantification of Complex Systems -Part II of III Brighton 1 MS20 Advances in Variational Methods and Applications to Materials - Part II of III Brighton 2 **CP1** Wave Mechanics Brighton 3 **CP2** Microstructural Mechanics Brighton 4

3:45 p.m. – 4:15 p.m. Coffee Break *Grand Station Ballroom 3-5*

Sunday, May 19

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4:15 p.m. - 6:15 p.m. **Concurrent Sessions** MS21 Advances in Mathematical and Numerical Techniques for Electronic Structure Calculations -Part III of III Grand Station Ballroom 1-2 MS22 Mechanics and Physics of Growth in Soft and Hard Materials - Part III of III Haselton 1 & 2 MS23 Emergent Properties in Metamaterials and Extreme Wave-phenomena: Analysis, Design, Modeling - Part III of III Woodlawn 1 MS24 Defects in Complex Materials: Interplay between Theory and Computation - Part III of III Pointsview MS25 Transforming Materials and Structures - Part III of IV Ellwood 1 MS26 Machine-learning-enabled Materials' Design - Part III of III Edenburg MS27 Theoretical and Applied Aspects of Nonlocal Models - Part III of III Stoops Ferry MS28 Advances in Probabilistic Methods for Uncertainty Quantification of Complex Systems -Part III of III Brighton 1 MS29 Advances in Variational Methods and Applications to Materials - Part III of III Brighton 2 MS30 CANCELLED-Multiphase and Multiscale Systems in Materials Science: Analysis and Simulation Brighton 3 MS31 Interaction of Solid Mechanics and Mathematics: Modelling, Analysis and Applications - Part II of II Brighton 4

6:15 p.m. – 6:30 p.m. Intermission

6:30 p.m. – 8:30 p.m. PP1 Reception and Poster Session *Reflections*

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Monday, May 20

7:00 a.m. - 6:15 p.m.

Registration Grand Station Ballroom 3 Foyer

8:00 a.m. – 8:45 a.m.

IP2 Liquid Crystal Polymeric Networks: Modeling, Approximation, and Computation Ricardo Nochetto, University of Maryland, College Park, U.S. *Grand Station Ballroom 1-2*

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8:45 a.m. – 9:30 a.m.

IP3 Characterizations of Symmetric Polyconvexity and Applications in Geometrically Linear Theory of Elasticity Anja Schlomerkemper, Universität Würzburg, Germany *Grand Station Ballroom 1-2*

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9:30 a.m. – 10:00 a.m. Coffee Break *Grand Station Ballroom 3-5*

10:00 a.m. – 12:00 p.m. Concurrent Sessions

MS32 Nonequilibrium Quantum Dynamics and Applications - Part I of IV Haselton 1 & 2 MS33 Transforming Materials and Structures - Part IV of IV Ellwood 1 MS34 Accelerating Analysis and Design of Complex Materials via Novel Numerical Methods and Machine Learning Techniques - Part I of II Brighton 4 MS35 Computational and Analytical Advances in Nonlocal Modeling - Part I of II Brighton 3 MS36 Material Design Supported by the NSF DMREF Program - Part I of II Grand Station Ballroom 1-2 MS37 Mathematical and Computational Aspects of Multiscale Materials Structures: Advances and New Trends - Part I of III Brighton 2 MS38 Analysis and Modeling of Gradient Flows with Multiscale Effects - Part I of III Edenburg MS39 The Statistical Nature of Metallic Material Deformation Leading to Damage Events - Part I of III Stoops Ferry MS40 Analysis, Homogenization, and Spectral Problems in Materials Science - Part I of V Brighton 1

MS41 Programmable Assembly: Inverse Design of Materials from Discrete Components - Part I of V *Pointsview*

Monday, May 20

MS42 Emerging Trends in Multiscale Modeling, Analysis and Simulation of Problems in Materials Science - Part I of IV *Woodlawn 1*

12:00 p.m. – 1:30 p.m. Lunch Break

1:30 p.m. – 2:15 p.m.

IP4 Defects at Grain Boundaries: at the Frontiers of Variational Analysis for Material Defects Adriana Garroni, Universita di Roma "La Sapienza," Italy *Grand Station Ballroom 1-2*

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2:30 p.m. – 4:30 p.m.

Concurrent Sessions

MS43 Nonequilibrium Quantum Dynamics and Applications - Part II of IV Haselton 1 & 2 MS44 Mechanical Metamaterials: Recent Advances in Modeling, Computation, and Experiment - Part I of IV Ellwood 1 MS45 Accelerating Analysis and Design of

Complex Materials via Novel Numerical Methods and Machine Learning Techniques - Part II of II Brighton 4

MS46 Computational and Analytical Advances in Nonlocal Modeling - Part II of II *Brighton 3*

MS47 Material Design Supported by the NSF DMREF Program - Part II of II

Grand Station Ballroom 1-2

MS48 Mathematical and Computational Aspects of Multiscale Materials Structures: Advances and New Trends - Part II of III

Brighton 2

MS49 Analysis and Modeling of Gradient Flows with Multiscale Effects - Part II of III

Edenburg

MS50 The Statistical Nature of Metallic Material Deformation Leading to Damage Events - Part II of III

Stoops Ferry CP3 Phase-Field Methods Brighton 1 CP4 Mechanics of Functional Materials Ellwood 1

4:30 p.m. – 5:00 p.m. Coffee Break

Grand Station 3-5

5:00 p.m. – 7:00 p.m.

Concurrent Sessions MS51 Nonequilibrium Quantum Dynamics and Applications - Part III of IV Haselton 1 & 2

Monday, May 20

MS52 Mechanical Metamaterials: Recent Advances in Modeling, Computation, and Experiment - Part II of IV

Ellwood 1

MS53 Machine Learning's Role in Uncovering Insights from Heterogeneous Materials Data - Part I of II

Grand Station Ballroom 1-2

MS54 Mathematical and Computational Aspects of Multiscale Materials Structures: Advances and New Trends - Part III of III

Brighton 2

MS55 Analysis and Modeling of Gradient Flows with Multiscale Effects - Part III of III *Edenburg*

MS56 The Statistical Nature of Metallic Material Deformation Leading to Damage Events - Part III of III

Stoops Ferry

MS57 Analysis, Homogenization, and Spectral Problems in Materials Science - Part II of V *Brighton 1*

MS58 Programmable Assembly: Inverse Design of Materials from Discrete Components - Part II of V *Poinsview*

MS59 Emerging Trends in Multiscale Modeling, Analysis and Simulation of Problems in Materials Science - Part II of IV

Woodlawn 1

MS60 Variational and Geometric Methods for Curvature and Elasticity - Part I of II

Brighton 4

MS61 Recent Advances and New Trends in Phase Field Modeling - Part I of III *Brighton 3*

Tuesday, May 21

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7:00 a.m. – 4:15 p.m.

Registration Grand Station Ballroom 3 Foyer

8:00 a.m. – 8:45 a.m.

IP5 Integral Systems for Electron Kinetic Transport Mean Field Theory Problems Applied to Plasmas in Solid States and Soft Condensed Matter Irene M. Gamba, University of Texas, U.S. *Grand Station Ballroom 1-2*

8:45 a.m. – 9:30 a.m.

IP6 Quantum-accurate Large-Scale Atomistic Simulation of Materials with LAMMPS and FitSNAP* Aidan Thompson, Sandia National Laboratories, U.S. *Grand Station Ballroom 1-2*

Tuesday, May 21

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9:45 a.m. - 10:15 a.m.

Coffee Break Grand Station Ballroom 3-5

10:00 a.m. - 12:00 p.m.

Concurrent Sessions MS62 Nonequilibrium Quantum Dynamics and Applications - Part IV of IV Haselton 1 & 2 MS63 Mechanical Metamaterials: Recent Advances in Modeling, Computation, and Experiment - Part III of IV Elwood 1 MS64 Machine Learning's Role in Uncovering Insights from Heterogeneous Materials Data - Part II of II Grand Station Ballroom 1-2 MS65 Analysis, Homogenization, and Spectral Problems in Materials Science -Part III of V Brighton 1 MS66 Programmable Assembly: Inverse Design of Materials from Discrete Components - Part III of V Pointsview MS67 Emerging Trends in Multiscale Modeling, Analysis and Simulation of Problems in Materials Science - Part III of IV Woodlawn 1 MS68 Variational and Geometric Methods for Curvature and Elasticity - Part II of II Brighton 4 MS69 Recent Advances and New Trends in Phase Field Modeling - Part II of III Brighton 3 MS70 Topological Soft Matter - Part I of III Woodlawn 1 MS71 Reduced Modeling and Computations in Mathematical Materials Science - Part I of III Edenburg MS72 Using Uncertainty Quantification to Improve Learning in Atomistic Modeling Brighton 2

12:00 p.m. – 1:30 p.m. Lunch Break

1:30 p.m. – 2:15 p.m.

IP7 Advances in Massively Parallel Electronic Structure Calculations Based on High-Order Finite Difference Approaches Leeor Kronik, Weizmann Institute of Science, Israel *Grand Station Ballroom 1-2*

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2:45 p.m. – **3:15 p.m.** Coffee Break *Grand Station Ballroom 3-5*

Tuesday, May 21

..... 2:45 p.m. - 4:45 p.m. **Concurrent Sessions** MT1 Multi-Modal Data Driven and Physics-Informed Machine Learning with Uncertainty for Materials Applications Woodlawn 1 MS73 Advances in Modeling and Simulations for 2D Quantum Materials - Part I of II Brighton 4 MS74 Mechanical Metamaterials: Recent Advances in Modeling, Computation, and Experiment - Part IV of IV Ellwood 1 MS75 Thin Structures: at the Intersection of Analysis, Numerics, and Physics - Part I of IV Ellwood 1 MS76 Role of Numerics and Optimization in Materials Science - Part I of III Edenburg MS77 Analysis, Homogenization, and Spectral Problems in Materials Science - Part IV of V Brighton 1 MS78 Programmable Assembly: Inverse Design of Materials from Discrete Components - Part IV of V Pointsview MS79 Emerging Trends in Multiscale Modeling, Analysis and Simulation of Problems in Materials Science - Part IV of IV Woodlawn 1 MS80 Mechanics of Defects in Hard and Soft Materials - Part I of IV Haselton 1 & 2 MS81 Recent Advances and New Trends in Phase Field Modeling - Part III of III Brighton 3 CP5 Mechanics of Soft and Fluidic Systems

Wednesday, May 22

7:00 a.m. – 4:15 p.m. Registration *Grand Station Ballroom 3 Fover*

8:00 a.m. – 8:45 a.m.

Brighton 2

IP8 Surrogate Modeling in Multiscale Computing Jaroslaw Knap, U.S. Army Research Laboratory, U.S.

Grand Station Ballroom 1-2

8:45 a.m. – 9:30 a.m.

IP9 A New Class of Numerical Methods with Computational Intelligence for Materials Processing and Layered Additive Manufacturing Arif Masud, University of Illinois Urbana-Champaign *Grand Station Ballroom 1-2*

Wednesday, May 22

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9:45 a.m. – 10:15 a.m. Coffee Break *Grand Station 3-5*

10:00 a.m. - 12:00 p.m. **Concurrent Sessions** MS82 Advances in Modeling and Simulations for 2D Quantum Materials - Part II of II Brighton 2 MS83 Thin Structures: at the Intersection of Analysis, Numerics, and Physics - Part II of IV Grand Station Ballroom 1-2 MS84 Role of Numerics and Optimization in Materials Science - Part II of III Edenburg MS85 Analysis, Homogenization, and Spectral Problems in Materials Science - Part V of V Brighton 1 MS86 Programmable Assembly: Inverse Design of Materials from Discrete Components - Part V of V Pointsview MS87 Mechanics of Defects in Hard and Soft Materials - Part II of IV Haselton 1 & 2 MS88 Topological Soft Matter - Part II of III Woodlawn 1 MS89 Analytical and Computational Methods in Models of Soft Matter - Part I of III Brighton 3 MS90 Reduced Modeling and Computations in Mathematical Materials Science - Part II of III Ellwood 1 MS91 Computational Methods and Machine Learning Accelerated Algorithms for Phase-Field Modeling - Part I of II Stoops Ferry MS92 Computational Geometry and Graph Theory for Crystalline Materials - Part I of II Brighton 4

12:15 p.m. – 2:00 p.m. Lunch Break

1:30 p.m. – 2:15 p.m. IP10 Boundary Defects in Liquid Crystals Lia Bronsard, McMaster University, Canada *Grand Station Ballroom 1-2*

2:45 p.m. – **3:15 p.m.** Coffee Break *Grand Station Ballroom 3-5*

2:45 p.m. – 4:45 p.m. Concurrent Sessions MT2 Numerical and Mathematical Aspects of Nonlocal Models for Fracture *Brighton 1*

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Wednesday, May 22

Thursday, May 23

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MS93 Thin Structures: at the Intersection of Analysis, Numerics, and Physics - Part III of IV Grand Station Ballroom 1-2 MS94 Role of Numerics and Optimization in Materials Science - Part III of III Edenburg MS95 Mechanics of Defects in Hard and Soft Materials - Part III of IV Haselton 1 & 2 MS96 Topological Soft Matter - Part III of III Woodlawn 1 MS97 Analytical and Computational Methods in Models of Soft Matter - Part II of III Brighton 3 MS98 Reduced Modeling and Computations in Mathematical Materials Science - Part III of III Ellwood 1 MS99 Computational Methods and Machine Learning Accelerated Algorithms for Phase-Field Modeling - Part II of II Stoops Ferry MS100 Light and Matter - Part I of II Pointsview MS101 Mathematical Modeling of Microstructural Materials - Part I of II Brighton 2 CP6 Data Driven and Related Methods Brighton 4

4:45 p.m. – 5:00 p.m. Intermission

5:00 p.m. - 6:00 p.m.

SIAG/MS Business Meeting. Complimentary beer and wine will be served. Grand Station Ballroom 1-2

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7:30 a.m. – 1:30 p.m. Registration *Grand Station Ballroom 3 Foyer*

8:00 a.m. – 8:45 a.m.

IP11 Homogenization for Soft Composite Materials Pedro Ponte Castaneda, University of Pennsylvania, U.S. *Grand Station Ballroom 1-2*

8:45 a.m. - 9:30 a.m.

IP12 Title Not Available at Time of Publication Glaucio Paulino, Princeton University, U.S. *Grand Station Ballroom 1-2*

9:45 a.m. – 10:15 a.m.

Coffee Break Grand Station Ballroom 3-5

Grand Station Ballroom 3-5 10:00 a.m. – 12:00 p.m. **Concurrent Sessions** MS102 Thin Structures: at the Intersection of Analysis, Numerics, and Physics - Part IV of IV Grand Station Ballroom 1-2 MS103 Mechanics of Defects in Hard and Soft Materials - Part IV of IV Haselton 1 & 2 MS104 Analytical and Computational Methods in Models of Soft Matter - Part III of III Brighton 3 MS105 Mathematical Modeling of Microstructural Materials - Part II of II Brighton 2 MS106 Variational Methods in Material Science Ellwood 1 MS107 Computational Geometry and Graph Theory for Crystalline Materials - Part II of II Brighton 4 MS108 Light and Matter - Part II of II Pointsview **CP7** Nanoscale Mechanics Brighton 1 CP8 Other Topics Woodlawn 1 12:00 p.m. – 1:30 p.m. Lunch Break

1:30 p.m. – 1:45 p.m.

Closing Remarks Grand Station Ballroom 1-2

1:45 p.m. – 2:30 p.m. IP13 Intelligentsia of Nano-Architected Hierarchical Materials Julia Greer, California Institute of Technology, U.S. *Grand Station Ballroom 1-2*

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ABBREVIATION KEY

CP = Contributed Presentation Session IP = Invited Plenary Speaker MS = Minisymposium MT = Minitutorial PD = Panel Discussion PP = Poster Session

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Second Floor