

## Invited Talks of *The NOMAD Laboratory* since September 2022 to September 2025

### 2025

**Dey, Manoj:** Discovery of Novel Memristor Materials by Artificial Intelligence. AWASES Merck-Intel Workshop, Merck Headquarter, Darmstadt, Germany (Mar 2025)

**Foppa, Lucas:** Learning Rules for Catalyst Design via Artificial Intelligence. COST Workshop on ML/Computational Materials Science for Catalysis, Fraunhofer IWM, Freiburg, Germany (Feb 2025)

**Foppa, Lucas:** AI-Guided Workflows for the Discovery of Novel Materials. APS March Meeting 2025, Anaheim, United States (Mar 2025)

**Foppa, Lucas:** Modelling Materials' Properties via the "Materials Genes". CECAM Workshop, School on Machine Learning for Molecules and Materials Research, Zadar, Croatia (Jun 2025)

**Foppa, Lucas:** Describing Materials Properties and Functions via the "Materials Genes" Concept. Seminar at the Institute of Physics, University of Sao Paulo, Brazil (Jun 2025)

**Foppa, Lucas:** AI-Guided Workflows for Materials Design. Materials Informatic Workshop, CNPEM/ILUM-Max Planck meeting on electronic Structure methods and materials informatics, Campinas, Brazil (Jul 2025)

**Foppa, Lucas:** Assessing the Importance of Primary Features in SISO Models via Partial Effects, International Workshop on First-principles and Artificial-Intelligence Methods for Materials, Jülich, Germany (Sept 2025)

**Foppa, Lucas:** Explainable AI models for Materials Science with the SISO Approach, FHI-aims Webinar Series 2025, Online Event (Sept 2025)

**Green, James:** Demonstration on DFT - FHI-aims. 1st TIMES School, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany (Jun 2025)

**Nair, Akhil S.:** AI-Guided Discovery of Acid-Stable Oxides for Electrocatalysis, FHI-Workshop on Current Research Topics at the FHI. Potsdam, Germany (May 2025)

**Nair, Akhil S.:** Building Trust in Machine Learning Models with Uncertainty Quantification, International Workshop on First-principles and Artificial-Intelligence Methods for Materials, Jülich, Germany (Sept 2025)

**Ren, Xinguo:** New Features of the GW Implementation in LibRPA and Machine Learning the GW Self-Energy, International Workshop on First-principles and Artificial-Intelligence Methods for Materials, Jülich, Germany (Sept 2025)

**Scheffler, Matthias:** Density Functional Theory and Artificial Intelligence in Materials Science. Seminar of the Condensed Matter Theory Group, The University of Sydney, Sydney, Australia (Jan 2025)

**Scheffler, Matthias:** Artificial Intelligence in Materials Science. Colloquium at the School of Physics, the University of Sydney, Sydney, Australia (Jan 2025)

**Scheffler, Matthias:** Artificial Intelligence for Materials Science. DPG Meeting 2025, Focus Session on "Using Artificial Intelligence Tools in Magnetism", Regensburg, Germany (Mar 2025)

**Scheffler, Matthias:** Discovery of Novel Memristor Materials by Artificial Intelligence. AWASES Merck-Intel Workshop, Merck Headquarter, Darmstadt, Germany (Mar 2025)

**Scheffler, Matthias:** Artificial Intelligence for Materials Science. Physics Colloquium, University of Luxembourg, Luxembourg (Apr 2025)

**Scheffler, Matthias:** AI-Driven Discovery: Symbolic Regression Unveils Acid-Stable Oxides for Catalysis. Symposium on Frontiers in the Chemical Physics of Heterogeneous Interfaces and Beyond, Frick Chemistry Laboratory, Princeton University, Princeton, NJ, USA. (Jun 2025)

## 2024

**Foppa, Lucas:** Learning Design Rules for Heterogeneous Catalysts via Artificial Intelligence. Surface Science Discussions 2024, University of Poznan, Poland, Online Event (Jan 2024)

**Foppa, Lucas:** Towards a Multi-Objective Optimization of Subgroups for the Discovery of Materials with Exceptional Performance. APS March Meeting 2024, Minneapolis, United States (Mar 2024)

**Foppa, Lucas:** Multi-Objective Optimization of Subgroups for the Discovery of Exceptional Materials. Meeting 2024, Berlin, Germany (Mar 2024)

**Foppa, Lucas:** From Prediction to Action: Critical Role of Performance Estimation for Machine-Learning-Driven Materials Discovery. DPG Meeting 2024, Berlin, Germany (Mar 2024)

**Foppa, Lucas:** Design of Palladium-Based Alloys for the Catalytic Hydrogenation of Concentrated Acetylene via Mechanochemical Synthesis and Artificial Intelligence. DPG Meeting 2024, Berlin, Germany (Mar 2024)

**Foppa, Lucas:** AI-Model-Driven Optimization of Materials Properties: Challenges and Application to Catalyst Discovery. Symposium for the Max-Planck-Cardiff Centre on the Fundamentals of Heterogeneous Catalysis (FUNCAT), Cardiff University, Cardiff, United Kingdom (Apr 2024)

**Foppa, Lucas:** Identifying Materials Genes via Artificial Intelligence. FHI Workshop, Potsdam, Germany (Apr 2024)

**Foppa, Lucas:** Learning Design Rules for Heterogeneous Catalysis via AI. Chemistry Colloquium, Universidad Jaume I, Castellon, Spain (May 2024)

**Foppa, Lucas:** Learning Rules for Materials Design via AI. Future of Materials Discovery Workshop, University College London, London, United Kingdom (Jun 2024)

**Foppa, Lucas:** Identifying Rules Describing Materials Properties and Functions via Tailored Artificial Intelligence. Theoretical Chemistry Colloquium, Freie Universität Berlin, Berlin, Germany (Jun 2024)

**Foppa, Lucas:** Learning Rules for Catalyst Design via Artificial Intelligence. 1st International CCSS Workshop "Designing the Future of Electrocatalysis with Compositionally Complex Solid Solutions", Ruhr-Universität Bochum, Bochum, Germany (Aug 2024)

**Foppa, Lucas:** From Prediction to Action: Critical Role of Performance Estimation for Machine-Learning-Driven Materials Discovery. 5th MACSMIN meeting, Materials Innovation Factory, Liverpool, United Kingdom (Sept 2024)

**Foppa, Lucas:** Describing Materials Properties and Functions via the "Materials Genes" Concept. International Workshop on Data-Driven Computational and Theoretical Materials Design, Shanghai, China (Oct 2024)

**Foppa, Lucas:** Data-Centric Heterogeneous Catalysis: Identifying Materials Genes with Artificial Intelligence. 10th Symposium on Surface Science, Kita-kyushu, Japan (Oct 2024)

**Foppa, Lucas:** Describing Complex Materials Properties and Functions via the "Materials Genes" Concept. The IOP-HU Early Career Researcher Conference on Energising Materials 2024, CSMB, Berlin, Germany (Nov 2024)

**Hassanzada, Qaem:** Towards an *ab initio* kinetic Monte Carlo model for the growth of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> (100). DPG Meeting 2024, Berlin, Germany (Mar 2024)

**Kang, Kisung:** Active-Learning for Machine-Learned Interatomic Potentials; The Example of Strongly Anharmonic Materials. APS March Meeting 2024, Minneapolis, United States (Mar 2024)

**Kang, Kisung:** Active-Learning Training of Accurate Machine-Learned Interatomic Potentials for Strongly Anharmonic Materials. DPG Meeting 2024, Berlin, Germany (Mar 2024)

**Kang, Kisung:** Sustainable Thermoelectric Materials: First-Principles and Machine Learning Studies. The 2nd World Congress of Korean Scientists & Engineers, Seoul, South Korea (Jul 2024)

**Nair, Sugathan Akhil:** Leveraging Multi-Fidelity Data In AI-Driven Sequential Learning of Materials Properties: Identifying Stable Water Splitting Catalysts. DPG Meeting 2024, Berlin, Germany (Mar 2024)

**Ren, Xinguo:** Basis-Error Free RPA Correlation Energy for Atomic and Diatomic Systems Based on the Sternheimer Equation. CECAM-CN Workshop on Excited States and Dynamics in Condensed Phases, Beijing Computational Science Research Center, Beijing, China (May 2024)

**Ren, Xinguo:** Low-Scaling RPA and GW Methods Towards Large-Scale Systems Based on Numerical Atomic Orbitals. Symposium on Materials Theory, driven by Aphrodite, *ab initio* Computations, and Artificial Intelligence, Paphos, Cyprus (Nov 2024)

**Scheffler, Matthias:** AI-guided Workflows for Efficiently Screening the Materials Space. Physics Colloquium, University of California at San Diego San Diego, USA (Feb 2024)

**Scheffler, Matthias:** AI-guided Workflows for Efficiently Screening the Materials Space. Physics Colloquium, University Duisburg-Essen, Duisburg, Germany (Apr 2024)

**Scheffler, Matthias:** Open Science and AI: Künstliche Intelligenz für die Entdeckung neuer und neuartiger Materialien. Rotary Club Berlin unter den Linden, Berlin, Germany (Apr 2024)

**Scheffler, Matthias:** Open Data and Artificial Intelligence in Materials Science and Engineering: A new way of thinking research. Annual Magna Meeting, Rio de Janeiro, Brazil (May 2024)

**Scheffler, Matthias:** Exascale-critical Advancements in the FHI-aims Software. NOMAD Coe Final Review Meeting, Online Event (Jun 2024)

**Scheffler, Matthias:** Impact, Uncertain Expectations, and Open Challenges of AI in Materials Science. Plenary talk at Conference of Condensed Matter Physics (CCMP), Yangtze River Delta Physics Research Center, Liyang, China (Aug 2024)

**Scheffler, Matthias:** Conclusion of the Conference and Outlook for the Field. International Workshop on Data-Driven Computational and Theoretical Materials Design, Shanghai, China (Oct 2024)

**Scheffler, Matthias:** The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society. Colloquium at School of Physics and Information Technology, Shaanxi Normal University, Xi'an, China (Oct 2024)

**Scheffler, Matthias:** Density Functional Theory and Artificial Intelligence in Materials Science. Meeting at Synfuels China, Beijing, China (Oct 2024)

**Scheffler, Matthias:** Artificial Intelligence in Materials Science: Impact, Uncertain Expectations, and Open Challenges. Colloquium at the School of Physics, Peking University, Beijing, China (Oct 2024)

**Scheffler, Matthias:** Data-Centric Materials Science. 15th International Symposium on Atomic Level Characterizations for New Materials and Devices '24, Matsue, Shimane, Japan (Nov 2024)

## 2023

**Aggoune, Wahib:** Designing new memristor materials. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Rivera Arrieta, Herzain I.:** Identifying outstanding materials through exceptional model mining. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Foppa, Lucas:** Identifying Rules and Materials Genes of Heterogeneous Catalysis via Artificial Intelligence. Seminar of the School of Chemistry, University of Nottingham, Nottingham, UK (Mar 2023)

**Foppa, Lucas:** Identifying “Catalyst Genes” with Artificial Intelligence. Workshop on Multiscale Modelling of Materials and Surfaces, Lake District, UK (Apr 2023)

**Foppa, Lucas:** Subgroup Discovery Tutorial. School on Artificial Intelligence for Materials Science in the Exascale Era. Platja D’Aro, Spain (May 2023)

**Foppa, Lucas:** Identifying Materials Genes of Properties and Functions via AI. BigMax (Max Planck Research Network on Big-Data-Driven Materials Science), Grand Finale Workshop, Platja D’Aro, Spain (May 2023)

**Foppa, Lucas:** Data-Centric Materials Science: Identifying “Materials Genes” with AI. Seminar of the Institute of Materials Chemistry, TU Wien, Vienna, Austria (Jun 2023)

**Foppa, Lucas:** The “Genes” of Materials Properties and Functions Identified by Symbolic Regression. Summer School of the Center for Scalable Data Analytics and Artificial Intelligence, TU Dresden, Dresden, Germany (Jul 2023)

**Foppa, Lucas:** Beyond a Single Description in Subgroup Discovery of Exceptional Materials: Coherent Collections of Rules Clustered by Similarity. NOMAD Workshop, Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Foppa, Lucas:** The “Catalyst Genes” Identified by Artificial Intelligence. 22nd Brazilian Congress of Catalysis, Bento Gonçalves, Brazil (Sep 2023)

**Foppa, Lucas:** Identifying Rules and Materials Genes of Properties and Functions via AI. IOP-FHI Workshop on the Frontiers of Electronic Structure Theory and Materials Genomics, Beijing, China (Oct 2023)

**Foppa, Lucas:** Learning rules for selective hydrogenation catalysis with AI. Symposium for the Max-Planck-Cardiff Centre on the Fundamentals of Heterogeneous Catalysis (FUNCAT), MPI für Kohlenforschung, Mülheim an der Ruhr, Germany (Nov 2023)

**Foppa, Lucas:** Identifying Rules and Materials Genes of Properties and Functions via Tailored Artificial Intelligence. Theoretical Chemistry Colloquium, Humboldt-Universität zu Berlin, Germany (Dec 2023)

**Miyazaki, Ray:** Identifying Materials Genes Describing Selectivity of Catalytic CO<sub>2</sub> Hydrogenation: an AI Approach with Theoretical and Experimental Data. FUNCAT Symposium, Cardiff, UK (Mar 2023)

**Moerman, Evgeny:** Affordable and highly accurate coupled-cluster band gaps in the thermodynamic limit. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Nair, Sugathan Akhil:** Multi-Fidelity Modelling for Materials Discovery with Sequential Learning. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Purcell, Thomas A. R.:** Accelerating the High-Throughput Search for new Thermal Insulators. Special Seminar Series, University of Arizona, USA (Jan 2023)

**Purcell, Thomas A. R.:** Symbolic Regression and Explainable AI. School on Artificial Intelligence for Materials Science in the Exascale Era. Platja D’Aro, Spain (May 2023)

**Purcell, Thomas A. R.:** Accelerating the High-Throughput Search for new Thermal Insulators. School on Artificial Intelligence for Materials Science in the Exascale Era. Platja D’Aro, Spain (May 2023)

**Purcell, Thomas A. R.:** Recent advances in the SISO method and their implementation in the SISO++ code. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Ren, Xinguo:** Basis-Set-Error Free RPA Correlation Energy for Atomic and Diatomic System Based on the Sternheimer Equation, FHI-aims Developers' and Users' Meeting 2023, Hamburg, Germany (Aug 2023)

**Ren, Xinguo:** Advanced Electronic-Structure Methods Based on Numerical Atomic Orbitals: Basics and Recent Progress, Shanghai Institute of Applied Physics (SINAP), China, Shanghai (Nov 2023)

**Sbailo, Luigi:** Uncertainty quantification in deep neural networks to detect out-of-distribution samples. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Scheffler, Matthias:** Learning Rules and Identifying "Materials Genes" for Heterogeneous Catalysis by Artificial Intelligence. Modern Trends in Surface Science Studies, Poznan, Poland, Online Event (Jan 2023)

**Scheffler, Matthias:** The NOMAD Center of Excellence and The Max Planck Society. NOMAD Project Meeting, Vienna, Austria (Feb 2023)

**Scheffler, Matthias:** Finding "Rules" and "Genes" for Materials Properties and Functions by Artificial Intelligence. Fundamentals of Heterogeneous Catalysis: FUNCAT 2023, Cardiff, UK (Mar 2023)

**Scheffler, Matthias:** Learning Rules for High-Throughput Screening of Materials Properties and Functions. The Minerals, Metals, and Materials Society (TMS) General Meeting, San Diego, USA (Mar 2023)

**Scheffler, Matthias:** Finding "Rules" and "Genes" for Materials Properties and Functions by Artificial Intelligence. Duke Materials Initiative (DMI) Distinguished Lecture, Duke University, Durham, North Carolina, USA (Apr 2023)

**Scheffler, Matthias:** Electron-Vibrational Coupling in and beyond The Phonon Picture. Public Seminar of the Departments of Mechanical Engineering and Materials Science and Chemistry, Duke University, Durham, North Carolina, USA (Apr 2023)

**Scheffler, Matthias:** Efficient Discovery of Improved Energy Materials by an AI-guided Workflow: The Example of Thermal Conductivity. Workshop as part of the "Sino-German Mobility Program", Berlin-Dahlem, Germany (Aug 2023)

**Scheffler, Matthias:** Training Activities of the NOMAD CoE. NOMAD Project Meeting, Helsinki, Finland, (Aug 2023)

**Scheffler, Matthias:** Welcome and Overview, and The Role of Volker Heine for Computational Materials Science. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Scheffler, Matthias:** Efficient Discovery of Improved Energy Materials by an AI-guided Workflow: The Example of Thermal Conductivity. IOP-HU Early Career Researcher Conference on Condensed Matter Physics, Liyang, China (Oct 2023)

**Scheffler, Matthias:** Advancements in Exchange-Correlation Functionals for Ground and Excited States. IOP-FHI Workshop on the Frontiers of Electronic-structure Theory and Materials Genomics, Beijing, China (Oct 2023)

**Scheffler, Matthias:** Finding "Rules" and "Genes" for Materials Properties and Functions by Artificial Intelligence. IOP-CAS Daniel Tsui Distinguished Lecture, Institute of Physics/CAS, Beijing, China (Oct 2023)

**Scheffler, Matthias:** AI-guides Workflows for Efficiently Screening the Materials Space. MRS Fall meeting, Boston, USA (Oct 2023)

**Sobolev, Andrei:** Recent developments in GIMS. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Speckhard, Daniel:** Extrapolation of DFT results to the complete basis set limit. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Yao, Yi:** Performance Boosting Portable Acceleration of SISSO++ for Symbolic Descriptor Learning. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Zhang, Min-Ye:** GW Method for Periodic Systems Using Numeric Atom-Centered Orbitals. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Zhao, Shuo:** Anisotropic thermal conductivity studied with the *ab initio* Green-Kubo approach. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

**Zhou, Yuanyuan:** Replica-exchange Grand-Canonical method: surface restructuring and phase boundary at realistic conditions. NOMAD Workshop on Data-centric Cruising for New and Novel Materials, Mechanisms, and Insights, Kiel, Germany (Sep 2023)

## 2022 (from September)

**Rivera Arrieta, Herzain I.:** A data-centric approach for uncovering subgroups of active metal catalysts toward CO<sub>2</sub> activation. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Carbogno, Christian:** Heat and Charge Transport: Past, Present, and Future Developments. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Foppa, Lucas:** Hierarchical Symbolic Regression for Identifying Key Physical Parameters Correlated with Materials Properties. Seminar, Machine Learning School for Materials @ ILUM, Online Event (Sep 2022)

**Foppa, Lucas:** Identifying Materials Genes of Properties and Functions via Artificial Intelligence. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Foppa, Lucas:** Identifying Materials Genes of Properties and Functions via Artificial Intelligence. DPG Meeting of the Condensed Matter Section (SKM) 2022, Regensburg, Germany (Oct 2022)

**Ghiringhelli, Luca M.:** FAIRmat: Concept and News. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Kokott, Sebastian:** FHI-aims: The *ab initio* Materials Simulation Package. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Langer, Marcel:** Heat Flux for Machine Learning Potentials. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Leitherer, Andreas:** Crystal-structure identification via artificial intelligence. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Lion, Konstantin:** Surface stability of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> at realistic temperature and pressure conditions. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Miyazaki, Ray:** AI with Experimental and Theoretical Data toward the Understanding of CO<sub>2</sub> Hydrogenation Catalysis: The Role of the Supporting Materials. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Moerman, Evgeny:** An Open-source Interface to MP2 and Coupled-Cluster Methods for Solids for Localized Basis Set Codes. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Nafchi, Somayeh Faraji:** AI-driven discovery of transition-metal alloy catalysts for selective hydrogenation of acetylene to ethylene. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Purcell, Thomas A. R.:** AI Accelerated Workflows for Finding Thermal Insulators. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Purcell, Thomas A. R.:** Accelerating the High-Throughput Search for new Thermal Insulators with Symbolic Regression. Meeting on Overcoming the Global Energy Crisis by Materials Research Regional Series III, Georgia Institute of Technology, USA (Dec 2022)

**Quan, Jingkai:** Electronic-Transport Theory: Challenges and Solutions. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Quan, Jingkai:** *Ab initio* Theory of Electronic-Transport for Strongly Anharmonic Materials. Evaluation of the Max Planck Graduate Center for Quantum Materials, Max Planck Institute for Solid State Research, Stuttgart, Germany (Nov 2022)

**Ren, Xinguo:** Advanced *Ab-initio* Electronic Structure Calculations Based on Numerical Atomic Orbitals: Recent Progress and Future Perspectives. The 23rd Asian Workshop on First-Principles Electronic Structure Calculations, National Cheng Kung University, Tainan, Taiwan, Online Event (Oct 2022)

**Rossi, Mariana:** Recent Research Highlights from the Sabia Group. Theoretical Chemistry Seminar, University of Cambridge, Cambridge, UK (Nov 2022)

**Rossi, Mariana:** Quantum Mechanics for Electrons and Nuclei to Larger Scales. Theoretical and Physical Chemistry Seminar, University of Basel, Basel, Switzerland (Nov 2022)

**Rossi, Mariana:** Recent Research Highlights from the Sabia Group. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Sbailo, Luigi:** The NOMAD Artificial-Intelligence Toolkit and materials-science data visualization. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Scheffler, Matthias:** New and Novel Materials, Mechanisms, and Insights. NOMAD Meeting: Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective). Berlin-Griebnitzsee, Germany (Oct 2022)

**Scheffler, Matthias:** Materials Genes (Atomic-level Characterization) of Materials Properties and Functions. ALC '22: 14th International Symposium on Atomic Level Characterizations for New Materials and Devices '22, Bankoku Shinryokan, Okinawa, Japan (Oct 2022)

**Scheffler, Matthias:** Data-centric Research in the Natural Sciences. Berlin Science Week/Falling Walls, Workshop of the Berlin-Brandenburg Academy of Sciences and Humanities (BBAW), Berlin-Mitte, Germany (Nov 2022)

**Speckhard, Daniel:** Extrapolation to complete basis-set limit in density-functional theory by quantile random-forest models. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)

**Zhou, Yuanyuan:** *Ab initio* description of surface restructuring and phase boundary under realistic conditions. NOMAD Meeting, Revealing New and Novel Materials, Mechanisms, and Insights (a Perspective), Potsdam, Germany (Oct 2022)