Wednesday April 2 AGENDA

	Materials Innovation
	VIRTUAL ONLY
9:00 AM EST	Faster Mesoscale Model Building: What's New in Materials Studio 2025 **James Wescott**, Sr. Product Manager, BIOVIA
9:20 AM EST	Advances in Materials Studio 2025: Introducing Machine Learned Potentials **James Wescott**, Sr. Product Manager, BIOVIA
9:40 AM EST	Foundation Models and its Refinement for Materials and Molecules **Prof. Gabor Csanyi**, University of Cambridge
10:00 AM EST	Exploring Glass Transition in Polyethylene via MD: From Bulk to Isolated Chain **Armand Soldera, Prof., Ph.D., D.h.c.** Dean, Université de Sherbrooke
10:20 AM EST	COSMO-RS in formulation: past, present and future **Théophile Gaudin**, User Success Engineering Manager, BIOVIA
10:40 AM EST	Fast, Accurate and Robust Molecular Quantum Chemistry: BIOVIA TURBOMOLE 2025 **Uwe Huniar** Sr. R&D Scientific Software Engineering Manager, BIOVIA
11:00 AM EST	Catalysis Fundamentals of Selective Hydrogenation of Aromatic Hydrocarbons with Molecular Modeling in Materials Studio **Prof. Simon Podkolzin** Stevens Institute of Technology
11:20 AM EST	Meet with BIOVIA Team & Live Q&A **Stephen Todd; James Wescott; Armand Soldera; Simon Podkolzin; Marc Meunier; JasonDeJoannis; Uwe Huniar; Théophile Gaudin; Frank Eckert; Jian-jieLiang**

ABSTRACTS

9:00 AM - 9:20 AM

Faster Mesoscale Model Building: What's New in Materials Studio 2025

James Wescott, Sr. Product Manager, **BIOVIA**

Phenomena occurring at the mesoscale influence the performance of most materials to some extent and coarse-grained models are often employed to simulate at the appropriate time and length scales. Structure building, bead allocations and forcefield typing can all be streamlined using the tools available in Materials Studio 2025 to decrease the time to solution. In this talk I will review some of the latest updates including a new bilayer construction tool for lipid and surfactant studies.

9:20 AM - 9:40 AM

Advances in Materials Studio 2025: Solver Development and MACE Learned Potentials

James Wescott, Sr. Product Manager, **BIOVIA**

In this talk I will review the latest updates to quantum and classical solver modules in Materials Studio 2025 including the first release of MACE Learned Potentials. In particular I will describe the new implementation of MACE-OFF23 and MACE-MP-0 to the Forcite module and consider new possibilities for leveraging these new classes of forcefield for materials research.

ABSTRACTS

9:40 AM - 10:00 AM

Foundation models and its refinement for materials and molecules

Prof. Gabor Csanyi, **University of Cambridge**

I will discuss the present status of foundation models for materials molecules, and preview what is like to come in the next year. This includes orders of magnitude increases in training data sets and explicit electrostatics.

10:00 AM - 10:20 AM

Exploring Glass Transition in Polyethylene via MD: From Bulk to Isolated Chain

Armand Soldera, Prof., Ph.D., D.h.c.
Dean, **Universitéde Sherbrooke**

We investigate the glass transition behavior of polyethylene (PE) in both bulk and isolated chains using molecular dynamics simulations. By combining simulated dilatometry, Arrhenius analysis, and trans-state evolution, we identify a glass transition domain characterized by distinct temperatures, revealing that isolated chains generally exhibit lower Tgs than bulk, except for one intrinsic temperature linked to dihedral energy barriers. These findings provide insight into polymer flexibility and the fundamental nature of glass transition temperatures in different environments.

ABSTRACTS

10:20 AM - 10:40 AM

COSMO-RS in Formulation: Past, Present and Future

Théophile Gaudin
User Success Engineering Manager, **BIOVIA**

COSMO-RS has proven effective for predicting thermodynamic properties of pure liquids and mixtures of small to medium-sized molecules, but formulations typically involve complex mixtures with unknown exact compositions, seemingly beyond COSMO-RS's capabilities. Nevertheless, experience demonstrates that through careful problem definition or minimal experimental input, COSMO-RS can successfully address consumer product formulation challenges, with this presentation exploring both current capabilities and potential future applications in this domain.

10:40 AM - 11:00 AM

Fast, Accurate and Robust Molecular Quantum Chemistry: BIOVIA TURBOMOLE 2025

Uwe Huniar
Sr. R&D Scientific Software Engineering Manager, **BIOVIA**

This talk will cover the latest advancements in BIOVIA TURBOMOLE, a leading quantum chemistry tool for highly accurate molecular simulations. Key topics include enhanced DFT and beyond-DFT methods, precise spectral predictions, reaction energy calculations, and molecular optical device simulations, highlighting its growing impact in research and industry.

ABSTRACTS

11:00 AM - 11:20 AM

Catalysis Fundamentals of Selective Hydrogenation of Aromatic Hydrocarbons with Molecular Modeling in Materials Studio

Prof. Simon Podkolzin
Stevens Institute of Technology

Complete or partial selective hydrogenation of aromatic hydrocarbons is required in the production of multiple and diverse commodity and specialty chemicals. However, adsorption and reaction mechanisms of aromatics on noble metals, which are common in hydrogenation catalyst formulations, are not well understood. In this study, reaction mechanisms for selective hydrogenation of aromatic hydrocarbons to cycloolefins and cycloalkanes over noble metal catalysts were studied at the molecular level by combining experimental kinetic and spectroscopic measurements with density functional theory calculations in the Materials Studio. Reactive intermediates were identified and related to catalytic activity and selectivity differences. More active and more selective catalyst formulations were developed, which enable a more efficient single-step selective hydrogenation process as a replacement of current commercial multistep technologies.