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BASEL CAMPUS' SEMINARS: NOVEMBER 27TH 2026

NOVARTIS CAMPUS | NOVARTIS PAVILLON
ST. JOHANNES-HAFEN-WEG 5, 4002 BASEL - CH

OPEN PARTICIPATIONS: FREE REGISTRATION* VIA EMAIL: ESSTEAM@EXCELSUS2S.COM *NECESSARY TO BE INCLUDED IN THE LIST OF PARTICIPANTS

MARCUS NEUMANN



Avant-Garde Materials Simulation GmbH, Scientific Director and Founder

Dr. M. A. Neumann holds a PhD in Physics from the University of Grenoble (F). In 1999 he joined Materials Simulation Ltd. in Cambridge (UK), and in 2002 founded Avant-garde Materials Simulation, dedicated to turning Crystal Structure Prediction (CSP) from an academic playground into a reliable engineering tool. Twenty years of pioneering milestones in collaboration with visionary customers — from the first solid-state dispersion correction to the landmark TRHu(ST) method— have made modern CSP a standard technique used by pharmaceutical companies. He is now investigating how CSP can benefit from recent developments in machine learning and artificial intelligence.

GRAHAME WOOLLAM



Novartis Pharma AG
Technical Research & Development,
Materials Science
Associate Director, Science & Technology

G. R. Woollam, PhD, FRSC, is Associate Director in Materials Science at Novartis, with more than 20 years' experience in crystallisation, solid form design and pharmaceutical development.
His work focuses on translating predictive approaches, particularly crystal structure prediction, into practical decisions in drug development. As a Royal Academy of Engineering Visiting Professor in Chemical & Process Engineering at University College London, he teaches and works at the interface of predictive modelling, materials science and process engineering to advance digital pharmaceutical manufacturing.

Predicting What Matters: A Decade of Advancing CSP for Pharmaceutical Development

Crystal structure prediction has evolved from a computational challenge into a practical tool for pharmaceutical development. Over the past decade, Marcus Neumann and Grahame Woollam have collaborated from complementary sides of that evolution. Marcus and AMS-GmbH. have advanced the computational science that makes increasingly sophisticated CSP possible, while Grahame's work has focused on making those predictions relevant to the decisions faced in pharmaceutical development. Their collaboration has helped extend CSP beyond static crystal energy rankings, including free energy calculations, hydrate stability, crystallisability and scalable cloud based prediction, while continually testing what these advances mean in an industrial setting.

In this joint seminar, they will reflect on that decade long journey from what can be predicted to what needs to be known. Looking forward, they will introduce the Relative Stability Framework, which brings this progression to a central question for modern CSP: which predicted structures actually matter? By connecting predicted landscapes with experimental evidence and development context, the framework provides a route from computational possibility to pharmaceutical relevance.

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