

# Institute Lecture



## Prof. Mark E. Tuckerman

New York University, USA

### ***Molecular simulation and Machine Learning as Routes to Exploring Structure and Phase Behavior in Atomic and Molecular Crystals***

@ 6:15 pm | March 15, 2019

Venue: L17, LHC



#### **About the talk:**

Organic molecular crystals frequently exist in multiple forms known as polymorphs. Structural differences between crystal polymorphs can affect desired properties, such as bioavailability of active pharmaceutical formulations, lethality of pesticides, or electrical conductivity of organic semiconductors. Crystallization conditions can influence polymorph selection, making an experimentally driven hunt for polymorphs difficult. Such efforts are further complicated when polymorphs initially obtained under a particular experimental protocol “disappear” in favor of another polymorph in subsequent repetitions of the experiment. Consequently, theory and computational can potentially play a vital role in mapping the landscape of crystal polymorphism. However, traditional theoretical methods face their own challenges, and new approaches are needed. In

this talk, I will show, by leveraging concepts from statistical mechanics in combination with techniques of molecular simulation and machine learning, a that new paradigm in crystal structure prediction may be emerging.

#### **About the Speaker:**

Prof. Mark Tuckerman is currently Professor of Chemistry and Mathematics at New York University. His research interests include the development of enhanced molecular dynamics and machine learning algorithms for predicting the conformational equilibria of complex molecules, the exploration of structure and polymorphism in molecular crystals, and the generation of full free-energy landscapes for these systems. He introduced rigorous methods for accelerating molecular dynamics simulations via multiple time stepping and has leveraged these in the simulation of quantum systems using the Feynman path integral formalism. Prof. Tuckerman's honors and awards include the Japan Society for the Promotion of Science Fellowship, the Friedrich Wilhelm Bessel Research Award from the Alexander von Humboldt Foundation, the Camille Dreyfus Teacher-Scholar Award, an NSF CAREER Award, and the NYU Golden Dozen Teaching Excellence Award, and the Sentinels of Science Award from Publons.

**All are invited to attend**  
Dean of Research and Development