IMS Seminar

Friday, February 2, 2024
1:00 PM, Science 1 - Room G01

**Snacks, coffee, and tea will be served beginning at 12:30 p.m.*

Dr. Shubham Sharma
Senior Scientist, Computational Materials Science
Pfizer Inc.
(Hosted by Dr. Steven L. Suib)

Unraveling Polymorphism - Computational Strategies in Pharmaceutical Research

Abstract: Computational based predictive and informatics-based tools to design and de-risk medicines have seen tremendous growth in the last decade and have been recently well-integrated within pharmaceutical research. Advanced computational tools employing first-principles electronic structure theory, molecular dynamics, data-driven modeling, and machine learning have been incorporated into workflows for both solid-state and formulation design. One of the common applications of computational tools within the pharmaceutical industry is to understand the risk of crystal polymorphism. Crystal Structure Prediction (CSP) has emerged as a pivotal resource in understanding the three-dimensional arrangement of molecules, aiding in the discovery of new polymorphs. By leveraging advanced atomistic and molecular modeling approaches together with machine learning techniques, CSP facilitates the identification of most stable and pharmaceutically desirable forms, thereby accelerating drug development. The informatics-based approaches, on the other hand, allow for rapid understanding of the potential risks of polymorphism through data mining, efficient retrieval, and analysis of vast amounts of structural information against a large dataset of solved experimental structures. The integration of such computational tools into pharmaceutical research holds great potential to expedite drug development process and mitigate risks associated with polymorphism. This presentation aims to bridge theory and practical application, highlighting how computational techniques can enhance our capacity to predict, analyze, and mitigate polymorphism, ensuring the production of safe and effective medicines.

Biography: Dr. Shubham Sharma is a Senior Scientist, Computational Materials Science at Pfizer Inc, USA. Dr Sharma currently co-leads the Solid Form Design Center (SFDC) at Pfizer for de-risking medicines and is also a subject matter expert in Crystal Structure Predictions. A chemical engineer, Dr Sharma earned his PhD in Chemical & Environmental Engineering in 2021 from Brown University, RI, USA. His PhD research focused on method development and application of computational modeling techniques in the field of electro-chemistry and heterogeneous catalysis. Followed by his PhD, Dr Sharma served as a postdoctoral fellow at the Lawrence Livermore National Laboratory, CA, US where he contributed to the field of electro-chemical dissolution, surface-corrosion, and machine learning techniques in spectroscopy. Dr Sharma joined Pfizer in 2022 and currently serves as subject matter expert for various modeling deliverables at the Materials Sciences division.

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