School of Molecular Sciences
Arizona State University

SMS 2023 P&T Seminar

Thursday Sept 7 | 1pm | Biodesign Auditorium

Recipes for marrying chemical physics with informatics to study biomolecular complexity

Molecular modeling of biomolecular assemblies exemplifies a disruptive area holding both promises and contentions. We will start with a brief story of simulating the first ever cell organelle in molecular details to find how nature has chosen survival fitness over efficiency of energy transfer as an evolutionary design (*Cell*, 2019; *JACS* 2020; *ACS Cent Sci* 2022). Despite such advances in large-scale computations, biophysical simulation continues to grapple with handling molecular diversity. So, we will employ deep learning approaches often used in Google searches, called the inception network, to marry interaction signatures from alphafold models and proteomics analysis with predictable patient outcomes (*Cell Med* 2021; *Cell Sys*, 2022). An application will highlight how molecular modeling is used at an industrial scale to de-risk vector-based vaccines for distribution across 194 countries (*Science Adv* 2021). We will see how transient interactions are difficult to predict, and path integrals with reinforcement learning offer a possible way to track diversity of dynamics (*NeurIPS*, 2022). We will end with how human-computer interactions can be used as a ploy for community building and invoking curiosity in learners (*IEEE* CogSIMA 2023).

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Abhishek Singharoy is an Assistant Professor at SMS and Biodesign Institute's CASD Center at ASU, and an Alliance Fellow at Mayo Clinic. He completed graduate studies from IU Bloomington and was a Beckman Fellow at UIUC prior to joining ASU in 2018. Together with a team of biophysicists, structural biologists and computational modelers, Singharoy studies how phenotypic adaptations (growth, immunogenicity and drug-resistance) emerge by tuning the energy transfer between hundreds of proteins embedded in cell membranes or the crowded interiors of cells.

**ZOOM option available: https://asu.zoom.us/j/84890997395*