

# Tanmoy Sanyal

Scientist, Computational drug design & Structural biology

## About

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## Molecular modeling

Rosetta  
openMM  
LAMMPS  
GROMACS  
IMP  
Modeller  
UCSF ChimeraX  
PyMOL  
VMD

## ML frameworks

PyTorch  
Tensorflow  
Tensorflow-probability  
PyMC3

## Workflows

Snakemake  
AWS Batch

## Languages

Python (+Cython) (~20000+ lines)  
Fortran-90 (~1000+ lines)  
C++ (~4000+ lines)  
Bash  
TCL

## Open Source

LAMMPS  
Local density potential  
  
nbspike  
Integrative epitope prediction  
  
IMP  
Crosslink guided domain  
discovery  
  
PDB-Dev deposition  
Structure of SMC5/6

## Education

**University of California Santa Barbara** 2013 - 2018  
Santa Barbara, CA, USA  
Ph.D Chemical Engineering  
*Graduate emphasis in Computational Science & Engineering (Parallel Computing & Numerical methods for ODEs / PDEs)*

**Indian Institute of Technology Kharagpur** 2008 - 2013  
Kharagpur, WB, India  
Masters and Bachelors of Technology (Hons.) integrated dual degree Chemical Engineering

## Research Experience

**Novo Nordisk Research Center Seattle** 2022 - Present  
Scientist, Computational drug discovery

- **Biologics Design:** Design of peptides and antibodies for rare endocrine disorders, and SAR (structure activity relationship) analysis based on PLMs (protein language models)
- **Scientific Software development:** Computational workflows for automating molecular model building and MD simulation of modified peptides, such as small molecule acylations or peptide-biopolymer conjugates.

**Department of Bioengineering, University of California San Francisco** 2019 - 2022  
Postdoctoral scholar, Andrej Sali lab

- **Protein structure modeling using chemical crosslinks:** Combined Homology models + chemical-crosslinks + cryo-EM data for protein complex structure modeling; graph sampling methods to extract domain information from crosslinks. Applications include SMC and DNA helicase protein families.
- **Computational mapping of nanobody epitopes:** Developed software to integrate chemical crosslinks with escape mutation data for protein-protein docking. Applications include epitope prediction of nanobodies on wild-type SARS-CoV-2 spike and variants.
- **Whole cell models:** Developed Bayesian Network models to combine continuum scale (pharmacokinetic), particle scale (Brownian dynamics) and network scale (enzyme pathways) models of the pancreatic beta-cell into build a proof-of-concept multimodal digital twin Served as software lead within the Pancreatic Beta-Cell consortium (collaborating across UCSF, USC, ShanghaiTech and HUJI)

**Chemical Engineering, University of California Santa Barbara** 2013 - 2018  
PhD candidate, Shell lab

- **Thesis:** Next-Generation Coarse-Grained Models for Molecular Dynamics Simulations of Fluid Phase Equilibria and Protein Biophysics Using the Relative Entropy
- **Coarse-graining algorithms for bulk liquids:** Introduced the local density potential for structurally and thermodynamically accurate coarse-grained MD simulations of liquid-liquid phase separation, which are relatively rare in the chemical engineering literature
- **Coarse-graining algorithms for protein folding:** Developed protein backbone models for (i) template-free folding of 200+ residue coarse-grained protein domains using MD simulations, and (ii) studying self-assembly in amyloidogenic peptides
- **High Performance Computing:** As system administrator, set up 144 core Linux (Rocks 6.2) cluster and wrote utilities for automating (i) network-attached-storage management, and (ii) conflict-free compute resource sharing between lab members.

## Research Interests

Protein design

Forcefield development

Amyloidogenic self assembly

Whole cell models

Bayesian networks

Variational inference

## Volunteer

### Peer-review

2019 - Present

Structure, Review of Scientific Instruments, Rapid Reviews Covid-19, Life, Biomolecules, International Journal of Molecular Sciences

### Graduate Simulation Seminar Series, University of California Santa Barbara

2014 - 2016

Co-founder

Conception, organization, public outreach and long-term funding support from ChE, Materials Science and Computer Science departments.

## Selected Publications

Highly synergistic combinations of nanobodies that target SARS-CoV-2 and are resistant to escape  
F.D. Mast, P.C. Fridy, N.E. Karen, J. Wang, E.Y. Jacobs, J.P. Olivier, T. Sanyal, et al, *eLife*, 2021

Bayesian metamodeling of complex biological systems across varying representations  
B. Raveh, L. Sun, K.L. White, T. Sanyal, et al, *PNAS*, 2021

Integrative analysis reveals unique structural and functional features of the Smc5/6 complex  
F.D. Mast, P.C. Fridy, N.E. Karen, J. Wang, E.Y. Jacobs, J.P. Olivier, T. Sanyal, et al, *PNAS*, 2021

A hybrid, bottom up, structurally-accurate, Go-like coarse-grained protein model  
T. Sanyal, J. Mittal & M. Scott Shell, *JCP*, 2019

Transferable coarse-grained models of liquid-liquid equilibrium using local density potentials optimized with the relative entropy  
T. Sanyal & M. Scott Shell, *JPC-B*, 2018

Coarse-grained models using local-density potentials optimized with the relative entropy:  
Application to implicit solvation  
T. Sanyal & M. Scott Shell, *JCP*, 2016

## Recent conference presentations

7th Annual Computational Drug Development for Biologics Summit, Boston, MA, USA  
(Talk): *Unpacking a workflow for automating protractor placement on peptides for enhanced half life*, Oct-2022

Indian Biophysical Society Meeting, Navi Mumbai, India  
(Talk): *Integrative modeling of higher order complexes from binary binding modes*, Apr-2022

Biophysical Society Annual Meeting, San Francisco, CA, USA  
(Talk): *Rigid body assignment in integrative determination of protein complex structures*, Feb-2022

PDB50: A special symposium celebrating the 50th anniversary of the Protein Data Bank, (virtual)  
(Poster): *Integrative modeling of the SMC5/6 complex*, May-2021

USC Brige Institute - Pancreatic Beta Cell Consortium Retreat, Catalina Island, CA, USA  
(Workshop): *Meta-modeling: Probabilistic graphical models and your data*, Nov-2019

Berkeley Mini Stat Mech Meeting, Berkeley, CA, USA  
(Poster): *Coarse-grained models for protein folding and self-assembly with the relative entropy*, Jan-2019

## Awards

### IUPAB best orgal presentation

2022

44th Indian Biophysical Society Meeting

### Technopreneurship Promotion Programme

2009

Ministry of Science and Technology, Govt. of India

Seed money for prototype scale-up of bioreactors for algal biodiesel generation

### Jagdis Bose National Science Talent Search (JBNSTS) fellowship

2009