ASPEN CENTER FOR PHYSICS
2018 WINTER CONFERENCE

Data-driven Discovery and Design in Soft and Biological Materials
January 7-13, 2018

Arrival Day: Sunday 7 January

5-7 pm Hosted reception at ACP

7-9 pm No-host dinner at Hickory House

Day 1: Monday 8 January

LEARNING AND DATA-DRIVEN DESIGN IN SELF-ASSEMBLY

8-8:45 am 1: **Juan de Pablo, University of Chicago** – "Improving Directed Assembly in Soft Matter Through Data Driven Approaches"

8:45-9:30 am 2: **Jasna Brujic, NYU** – "Mayonnaise Robots"

9:30-10 am **MORNING BREAK**

10-10:45 am 3: **Andrew Ferguson, University of Illinois** – "Programmed assembly of anisotropic patchy colloids by landscape engineering"

10:45-11:30 am 4: **Matthew Spellings, University of Michigan** – "Machine learning for crystal identification and discovery"

11:30 am – 4:30 pm **MID-DAY RECESS**
**** COFFEE + LIGHT SNACK PROVIDED @ 4 pm ****

4:30-5:15 pm 5: **Uyen Lieu, Nat. Inst. Adv. Ind. Sci. & Tech. (AIST)** – "Restructuring behavior of colloidal aggregates in simple shear flow"

5:15-6:00 pm 6: **Kiersten Ruff, Washington University** – CAMELOT: A machine learning approach for coarse-grained simulations of aggregation

6:00 pm + **DINNERS IN TOWN**

Day 2: Tuesday 9 January

DATA-ENABLED ADVANCES IN MOLECULAR SIMULATION

8-8:45 am 7: **Risi Kondor, University of Chicago** – "Learning atomic force fields: the significance of descriptors"

8:45-9:30 am 8: **Linfeng Zhang, Princeton** – "A deep learning paradigm for molecular

simulations”

9:30-10 am **MORNING BREAK**

10-10:45 am 9: **Roberto Covino, MPI Biophysics** – “iMapD: intrinsic Map Dynamics exploration for uncharted effective free energy surfaces”

10:45-11:30 am 10: **Erik Luijten, Northwestern University** – “TBA”

11:30 am – 4:30 pm **MID-DAY RECESS**
**** GROUP LUNCH ON MOUNTAIN AT 1 pm ****
**** COFFEE + LIGHT SNACK PROVIDED @ 4 pm ****

4:30-5:15 pm 11: **Stacy Copp, Los Alamos National Laboratory** – “Color by data-driven design of genomic DNA-stabilized silver clusters”

5:15-6:00 pm 12: **Teng Zhang, Syracuse University** – “Model reduction for morphing graphene and 3D printed polymer sheets”

6:00 pm + **DINNERS IN TOWN**

Day 3: Wednesday 10 January

MACHINE LEARNING IN ACTIVE MATTER AND BIOLOGY

8-8:45 am 13: **Jure Dobnikar, Institute of Physics Chinese Academy of Sciences** – “Modeling bacterial surface motility”

8:45-9:30 am 14: **Gerard Wong, UCLA** – “Potential problems for machine learning in innate immunity”

9:30-10 am **MORNING BREAK**

10-10:45 am 15: **Michael Hagan, Brandeis University** – “Analyzing data from simulations and experiments on active nematics”

10:45-11:30 am 16: **Ernest Lee, UCLA** – “Machine learning and membrane remodeling activity”

11:30 am – 4:30 pm **MID-DAY RECESS**
**** OPTIONS: X-C ski and lunch at Aspen Golf Course ****

4:30-5:30 pm **PHYSICS CAFÉ**
Amish Patel, University of Pennsylvania
Jasna Brujic, NYU

5:30-6:30 pm **PUBLIC LECTURE**
“Prediction and control of extreme events and unlikely phenomena, from

rogue waves to protein folding" – **Eric Vanden-Eijnden, NYU**

6:30 pm + **DINNERS IN TOWN**

Day 4: Thursday 11 January

DATA-DRIVEN CONTROL AND OPTIMAL DESIGN

8-8:45 am 17: **Eric Vanden-Eijnden, NYU** – "Geometric approach to optimal nonequilibrium control"

8:45-9:30 am 18: **Feliks Nuske, Rice University** – "Spectral Properties of Projected Dynamics"

9:30-10 am **MORNING BREAK**

10-10:45 am 19: **Kyle Hall, Temple University** – "Novel Visualizations: Tools for Data-Driven Science"

10:45-11:30 am 20: **Lorenzo Boninsegna, Rice University** – "Design of rigorous coarse grained models using dynamical information"

11:30 am – 4:30 pm **MID-DAY RECESS**
**** COFFEE + LIGHT SNACK PROVIDED @ 4 pm ****

4:30-5:15 pm 21: **Amish Patel, University of Pennsylvania** – "Understanding and How Soft Nanostructured Surfaces Perturb Solvation"

5:15-6:00 pm 22: **Hythem Sidky, Notre Dame** – "Learning free energy landscapes using artificial neural networks"

6:30 pm + **BANQUET AT ASPEN MEADOWS + BLOCK AWARD**
**** PLEASE ARRIVE PROMPTLY AT 6:30 PM ****

Day 5: Friday 12 January

BRAINSTORMING, BREAKOUT, AND WRAP

9-10:30 am **BREAKOUT GROUPS**
A. Integration of machine learning with experiment (Chair: Wong)
B. Novel algorithmic strategies and tool accessibility (Chair: Luitjen)
C. Data paradigms for guided and inverse design (Chair: Ferguson)

10:30-11 am **MORNING BREAK**

11 am – 12:30 pm **BREAKOUT REPORTS + CONFERENCE WRAP-UP**
CONFERENCE CLOSE