Ranjan Mannige, Ph.D.

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Strengths

`DOMAINS`: Health & life sciences, statistical mechanics, computational biology/chemistry, graph theory.
`SKILLS`: Machine learning, multi-scale simulation, bioinformatics, big data generation, applied math.
`CODING`: **Python** (Numpy, Pandas, Scipy, OpenCV), C++, JavaScript/HTML, simulation packages.

Experience

Senior Data Scientist, Healthcare & Life Sciences Consultant. KPMG, Atlanta, GA.   *2017–*
Leveraging healthcare and life sciences data to reduce morbidity and expenses.

Health Data Science Fellow. Insight Data Science, San Francisco, CA.   *2017–2017*
Developed Rx Machina.com: a machine-learning web-app to predict drug toxicity.

Postdoc. Lawrence Berkeley National Laboratory (Molecular Foundry), Berkeley, CA.   *2012–2017*
Studied virus bioinformatics, biomimetic structure prediction, and self assembly.

Postdoc, Associate. Harvard University (Chemistry Dpt.), Cambridge, MA.   *2010–2012*
Developed a spontaneous route for the origin of the first functional biomolecule.

External Graduate Student. University of Michigan (Chemistry Dpt.), Ann Arbor, MI.   *2008–2010*
Mentored students and developed the Periodic Table for Viruses.

Education

Ph.D., Scripps Research Institute (Molecular Biology Dpt.), La Jolla, CA.   *2004–2010*
Resolved virus capsid design principles using math & bioinformatics.

B.S., University of Houston (Biology & Biochemistry Dpt.), Houston, TX.   *2001–2004*
Developed a novel algorithm for finding disparate patterns within protein sequences.

Publications

* denotes corresponding author(s).

22. **Mannige RV*** (2018) The BackMAP python module: how a simpler Ramachandran number can simplify the life of a protein simulator. PeerJ 6:e5745 [link|pdf|GitHub].

21. **Mannige RV*** (2017) An exhaustive survey of regular peptide conformations using a new metric for backbone handedness (h). PeerJ 5:e3327 [link|pdf|GitHub].

20. Montiel-García DJ, **Mannige RV**, Reddy VS & Carrillo-Tripp M* (2016) Structure-based sequence analysis of viral and cellular protein assemblies. Journal of Structural Biology 196(3):299 [link|pdf].

19. **Mannige RV***, Kundu J & Whitelam S* (2016) The Ramachandran number: an order parameter for protein geometry. PLoS ONE 11(8):e0160023 [link|pdf].

18. **Mannige RV**⋆ & Whitelam S⋆ (2016) Predicting the outcome of the growth of binary solids far from equilibrium. Physical Review E 93:042136 [link | pdf].

17. Robertson EJ, Battigelli A, Proulx C, **Mannige RV**, Haxon TK, Whitelam S & Zuckermann RN⋆ (2016) Design, Synthesis, and Assembly of Peptoid Nanosheets. Accounts of Chemical Research 49:(3)379 [link | pdf].   Journal cover [link]; Most downloaded paper in January 2016 [link].

16. **Mannige RV**⋆, Haxton TK, Proulx C, Robertson EJ, Battigelli A, Butterfoss G, Zuckermann RN & Whitelam S⋆ (2015) Peptoid nanosheets exhibit a new secondary structure motif. Nature 526:415 [link | pdf].   Featured by C&E News [link], MRS [link], Berkeley Lab [link 1 | 2] and 18 news outlets [link 1 | 2].

15. **Mannige RV**⋆ (2015) Landscape of kinetically trapped binary assemblies. Journal of Chemical Physics 143:214902 [link | pdf].

14. Sue AC-H◗, **Mannige RV**◗, Deng H, Cao D, Wang C, Gándara F, Stoddart JF⋆, Whitelam S⋆ & Yaghi OM⋆ (2015) Two-component metal-organic framework displaying compositional robustness to solution constitution. Proceedings of the National Academy of Sciences 112(18):5591 [link | pdf].
◗: Equal contribution   Featured in Phys.org [link].

13. Haxton TK⋆, **Mannige RV**, Zuckermann RN & Whitelam S⋆ (2015) Modeling sequence-specific polymers using anisotropic coarse-grained sites allows quantitative comparison with experiment. Journal of Chemical Theory and Computation 11(1):303 [link | pdf].

12. **Mannige RV**⋆ (2014) Dynamic new world: refining our view of protein structure, function and evolution. Proteomes 2(1):128 [link | pdf].
Figure reused in textbook Introduction to Protein Science (3rd Ed), by A. Lesk, Oxford University Press

11. Hedges LO, **Mannige RV** & Whitelam S⋆ (2014) Growth of equilibrium structures built from a large number of distinct component types. Soft Matter 10(34):6404 [link | pdf].
Journal cover [link]; Featured as a "hot paper" of 2014 [link].

10. **Mannige RV**⋆ (2014) Origination of the protein fold repertoire from oily pluripotent peptides. Proteomes 2(2):154 [link | pdf].

9. Mirijanian DT, **Mannige RV**, Zuckermann RN & Whitelam S⋆ (2014) Development and use of an atomistic CHARMM-based forcefield for peptoid simulation. Journal of Computational Chemistry 35(5):360 [link | pdf].   Journal cover [link]; Featured by the DoD [link]; Designated "Important upcoming paper" [link].

8. **Mannige RV**⋆ (2013) Two modes of protein sequence evolution and their compositional dependencies. Physical Review E 87(6):062714 [link | pdf].

7. **Mannige RV**⋆, Brooks CL III & Shakhnovich EI (2012) A universal trend among proteomes indicates an oily last common ancestor. PLoS Computational Biology 8(12):e1002839 [link | pdf].
GenomeWeb.com paper of note [link].

6. May ER, Arora K, **Mannige RV**, Nguyen H & Brooks CL III (2011) Multiscale modeling of virus structure, assembly and dynamics. Chapter in Book: Computational Modeling of Biological Systems: From Molecules to Pathways ISBN 9781461421450 [link].

5. **Mannige RV**⋆ & Brooks CL III⋆ (2010) Periodic table of virus capsids: implications for natural selection and design. PLoS ONE 5(3):e9423 [link | pdf].
Discussed in: 1) Principles of Molecular Virology, Academic Press; 2) Nanomedicine, Elsevier.

4. **Mannige RV** (2010) Principles of virus capsid design. ProQuest Publishing ISBN 9781109683769 [link | submitted pdf].

3. **Mannige RV**⋆ & Brooks CL III⋆ (2009) Geometric considerations in capsid size-specificity, auxiliary requirements and buckling. <u>Proceedings of the National Academy of Sciences</u> 106(21):8531 [link|pdf].

2. **Mannige RV**⋆ & Brooks CL III⋆ (2008) Tilable nature of virus capsids and the role of topological constraints in natural capsid design. <u>Physical Review E</u> 77(5):051902 [link|pdf].
   Featured by the APS (Focus, 21:18. [link]).

1. **Mannige RV** & Pettitt BM (2004) P-PIDA: a long-range pattern detection algorithm for proteins. <u>University of Houston Library</u>, Senior Honors Thesis.
   Winner of the University of Houston Outstanding Senior Thesis Award.

Upcoming Publications
⋆ denotes corresponding author(s).

23. Mannige RV⋆. One, two ... life: How Information could drive the evolution of complex life. In preparation.

22. Mannige RV⋆. Is information a fundamental driving force? In preparation.

Conferences Chaired

Chair of the 252nd ACS National Meeting session "Designing functional biomaterials: connecting experiment with theory and simulation (COMP)". August 2016.

Co-chair/organizer of the Molecular Foundry annual symposium session "Soft Matter Assembly & Dynamics". August 2015.

Journals Refereed

• Nature Materials • JACS • J Phys Chem • PLoS Computational Biology • Genomics (BMC)

• Chem Comm (Royal Society of Chemistry) • Mol Based Math Biol • Artificial Life Journal (MIT)

Invited Talks

19. Design criteria of novel protein-mimetic polymers from simulation. 02/02/2017.
   Department of Chemical and Biomolecular Design, Johns Hopkins.

18. Peptoid nanosheets exhibit a new secondary structure motif. 08/21-25/2016.
   Designing functional biomaterials: connecting experiment with theory and simulation (COMP)
   252nd ACS National Meeting, Philadelphia, PA.

17. How did simple life, and then complex life, originate? A protein perspective. 03/14/2016.
   From Dynamics to Function and Back Again: Adventures in Simulating Biomolecules (COMP)
   251th ACS National Meeting, San Diego, CA.

16. From biomimetics to virus capsid assembly: using theory to arrive at molecular design criteria.
   The Biodesign Institute, Arizona State University, 12/11/2015.

15. Discovery of a possible symmetry chaperone in virus capsids. 10/28/2015.
   Special Molecular Foundry Seminar, Berkeley, CA.

14. Snakes on a plane: simulation reveals novel secondary structure in the peptoid nanosheet. 08/07/2015.
    9th Peptoid Summit, Berkeley Lab, CA.

13. Simulation reveals novel secondary structure in the peptoid nanosheet. 01/30/2015.
    Department of Chemistry (Stat Mech Seminar), University of California, Berkeley, CA.

12. Features and faults of a structurally characterized peptoid nanosheet. 08/26/2014.
    Session on 2D materials, Molecular Foundry Annual Meeting, Berkeley, CA.

11. A novel secondary structure discovered in a biomimetic material. 08/26/2014.
    Session on biomaterials, Molecular Foundry Annual Meeting, Berkeley, CA.

10. Design criteria of novel protein-mimetic polymers from simulation. 04/24/2014
    Joint Imperial College and Berkeley Lab meeting, Berkeley Lab, CA.

9. Design criteria of novel protein-mimetic polymers from simulation. 04/07/2014.
   Molecular Foundry NanoBio seminar, Berkeley Lab, CA.

8. Design criteria of novel protein-mimetic polymers from simulation. 04/03/2014.
   Molecular Foundry NanoTheory seminar, Berkeley Lab, CA.

7. Protein-mimetic materials for molecular recognition and catalysis. 07/23/2013.
   Defense Threat Reduction Agency, Springfield, VA (theory-experiment talk with Dr. Zuckermann).

6. The behavior of artificial assemblies from simulation. 01/25/2013.
   Molecular Foundry NanoTheory Seminar, Lawrence Berkeley National Laboratory, Berkeley, CA.

5. Using simple models to understand and predict complex biological phenomena. 01/31/2012.
   Molecular Foundry, Lawrence Berkeley National Laboratory (Berkeley Lab), CA.

4. Evolution and design criteria of molecular assemblies. 12/09/2009.
   Harvard University, Department of Chemistry, Cambridge, MA.

3. All viruses are not alike: relating "hexamer complexity" to spherical capsid existence. 09/05/2008.
   Scripps' Annual Student-Faculty Symposium, Bahia Resort, San Diego, CA.

2. Virus capsids and mathematical considerations. 09/07/2007.
   Scripps' Annual Student-Faculty Symposium, Bahia Resort, San Diego, CA.

1. Constraints and freedoms in virus capsids: a theoretical perspective. 08/09/2007.
   Mathematical Virology Workshop, International Centre for Mathematical Sciences, Edinburgh, UK.

Honors

Poster Prize (3rd place) at the Berkeley Mini Stat Mech meeting, UC Berkeley, January 2015

Atomistic Modeling of Peptoid Nanosensors Postdoctoral fellow (international search), 2012–present.

Center for Theoretical Biological Physics fellow, UC San Diego, 2006–10.

Fletcher Jones Foundation Fellowship, Los Angeles, CA, 2004–05.

Outstanding Senior Thesis Award, University of Houston (UH), 2004.

UH Department of Chemistry fellow at the Institute for Molecular Design, 2003–2004.

Natural Sciences & Mathematics McCammon endowed scholarship, UH, 2003–04.

Baylor College of Medicine's 2003 Summer Medical and Research Training fellow, Summer 2003.

Natural Science and Mathematics excellence scholarship, UH, 2001–02.

Research Mentor/Teaching/Volunteer

Undergraduate mentor (Tianyi Liu), UC Berkeley, CA. Spring 2015–Summer 2016.

Undergraduate mentor (Michael Tong), UC Berkeley, CA. Summer and Fall 2014.

Graduate mentor (Leela Velautham), UC Berkeley, CA. 2013-2014.

Undergraduate co-mentor (Aristotle Mannan), University of Michigan, Ann Arbor. Summer 2009.

Volunteer instructor at the Educate the Rural science fair at Akluj, India. 2000.

Volunteer instructor of astronomy, Inter University Centre for Astronomy and Astrophysics. 2000.

Volunteer instructor at the National Science Day, IUCAA. 1999.

Volunteer Instructor as an IUCAA science public awareness team. 1998.