David R Bell, PhD

russell.bell567@gmail.com • 214-770-8265 • davidrussellbell.github.io

RESEARCH INTERESTS

My research interests lie in the area of computational chemistry and data science, particularly in developing innovative algorithms for generative multiscale modeling, molecular recognition, and error quantification to understand structure, higher-order assembly, and interaction of native and synthetic materials.

RESEARCH EXPERIENCE

Postdoctoral Researcher, Soft Matter Science Group 2017-2020
IBM T.J. Watson Research Center

- Implemented a machine learning-based pipeline to design immunotherapies using a crystallographic and MD simulation dataset
- Developed a multiscale model to study amyloid protein aggregation of an intrinsically-disordered protein based on an extensive molecular dynamics (MD) simulation dataset
- Developed a structure-based method to design RNAs for enhanced protein binding affinity using MD simulations, docking, free energy calculations, and bioinformatics tools
- Designed novel RNAs to bind a prominent cancer biomarker using the structure-based method with subsequent experimental confirmation of binding
- Investigated immune complex binding using MD simulations and free energy perturbation (FEP) calculations
- Explored lipid-coated quantum dot nanoparticle aggregation and aggregation-dependent toxicity of a widespread protein domain by MD simulation
- Characterized one-dimensional nanomaterials for methane and hydrogen gas storage
- Published research in *Cell, PNAS, JCP, PCCP, Nanoscale,* and presented at *ACS*

Research Assistant, Advisor: Pengyu Ren 2012-2017
University of Texas at Austin

- Developed a generative multiscale model for RNA structure prediction based on crystallographic structures and folding free energies
- Implemented the multiscale RNA model in the in-house molecular modeling software package TINKER with OpenMP parallelization
- Built a 2-D Brownian Dynamics model to study size and binding-interaction effects on reduced diffusion in a crowded membrane protein system
- Investigated an enhanced sampling free energy prediction method for the prediction of small-molecule binding in the community-wide drug-design competition, SAMPL4
- Performed periodic maintenance on the in-house Beowulf/GPU computing cluster
- Published research in *PCCP, Scientific Reports, JPCB, Soft Matter,* a book chapter, and presented the RNA research at *ACS* national meeting

TEACHING EXPERIENCE

Director, STEM Summer Camp 2019
IBM T.J. Watson Research Center

- Lead a summer science camp of 25 students age 12-13
- Designed teaching materials for all activities and courses including robotics, cyber security, polymers, and presentation skills
- Recruited and coordinated volunteers including school principals and camp counselors
- Organized and presented at on-site event to camp students and family members

Teaching Assistant 2013-2017
University of Texas at Austin

- Assisted a biomedical design course and an introductory computing course
- Worked with four student groups and collaborated with industrial partners to ensure completion of 1-year biomedical design projects
- Taught a computing lab course to reiterate and aid coursework completion

SKILLS

Programming: Python, Java, MATLAB, FORTRAN, C++
Modeling Software: OpenMM, NAMD, TINKER, GROMACS, AmberMD, VMD, PyMOL, AutoDock, DOT2, HOOMD
HPC Architectures: POWER8/9, Blue Gene Q, Intel x86

EDUCATION

Ph.D. Biomedical Engineering	University of Texas at Austin	Dec 2016
M.S. Biomedical Engineering	University of Texas at Austin	May 2015
B.S. Mechanical Engineering *summa cum laude*	Texas Tech University	May 2012

AWARDS AND HONORS

Outstanding Technical Achievement Award 2020
IBM T.J. Watson Research Center

David Bruton, Jr. Fellowhip— Graduate School 2016
University of Texas at Austin

Thrust 2000 Fellowship— Cockrell School of Engineering 2012-2016
University of Texas at Austin

Highest Ranking Graduate— Whitacre College of Engineering 2012
Texas Tech University

SERVICE

Instructor, STEM Summer Camp— IBM Research 2018-2019
CAD and bridge building activity, age 12-13

Instructor, Family Science Saturdays— IBM Research 2018-2019
Intro to electronics, children age 9-10 and parents

Judge, Science Fairs— New York City, Westchester County 2018-2019
Biochemistry, age 14-18

Volunteer, Westchester Land Trust— Westchester County 2017-2018
Maintenance of county lands and parks

SELECTED PUBLICATIONS # Citations: 352

D.R. Bell, J.K. Weber, W. Yin, T. Huynh, W. Duan, R. Zhou. 2019. *In silico* design and validation of high-affinity RNA aptamers targeting epithelial cellular adhesion molecule dimers. PNAS. 117: 8486-8493.

R. Ahmed, Z. Omidian, A. Giwa, B. Cornwell, N. Majety, **D.R. Bell**, S. Lee,…, R.Zhou, C. Jie, T. Donner, A.R.A. Hamid. 2019. A Public BCR Present in a Unique Dual-Receptor-Expressing Lymphocyte from Type 1 Diabetes Patients Encodes a Potent T Cell Autoantigen. Cell. 177: 1583-1599.

D.R. Bell*, S.-G. Kang*., T. Huynh, R. Zhou. 2018. Concentration-dependent binding of CdSe quantum dots on the SH3 domain. Nanoscale. 10: 351-358.

D.R. Bell, S. Y. Cheng, P. Ren. 2017. Capturing RNA Folding Free Energy with Coarse-Grained Molecular Dynamics Simulations. Scientific Reports. 7: 45812.

J.M. Obliosca, S. Y. Cheng, Y.-A. Chen, M. F. Llanos, Y.-L. Liu, D. M. Imphean, **D.R. Bell**, J. T. Petty, P. Ren, H.-C. Yeh. 2017. LNA Thymidine Monomer Enables Differentiation of the Four Single-Nucleotide Variants by Melting Temperature. Journal of the American Chemical Society. 139(20): 7110-7116.

D.R. Bell*, R. Qi*, Z. Jing*, J. Y. Xiang, C. Mejias, M. J. Schnieders, J. W. Ponder, P. Ren. 2016. Calculating binding free energies of host-guest systems using the AMOEBA polarizable force field. Physical Chemistry Chemical Physics. 18: 30261-30269.

J. R. Houser, D. J. Busch, **D.R. Bell**, B. Li, P. Ren, and J. C. Stachowiak. 2016. The Impact of Physiological Crowding on the Diffusivity of Membrane Bound Proteins. Soft Matter 12: 2127-2134.

D.R. Bell, Z. Xia, and P. Ren. RNA Coarse-Grained Model Theory. Many-body effects and electrostatics in multi-scale computation of biomolecules. Ed. Qian Cui, Markus Meuwly, and Pengyu Ren. Singapore: Pan Stanford Publishing, 2015.

Z. Xia, **D.R. Bell**, Y. Shi, and P. Ren. 2013. RNA 3D structure prediction by using a coarse-grained model and experimental data. The Journal of Physical Chemistry B 117(11):3135-3144.
(*Co-first authors)

SELECTED PRESENTATIONS

D.R. Bell, S.-G. Kang, R. Zhou. 2018. CdSe quantum dot aggregation-dependent toxicity on the SH3 domain. 256th ACS National Meeting & Exposition, Boston, Massachusetts. Presentation.

D.R. Bell, Z. Xia, P. Ren. 2015. Weighing energetics against best fit in RNA structure prediction. 249th ACS National Meeting & Exposition, Denver, Colorado. Poster.

D.R. Bell, P. Selokar, and T. D. Lillian. 2012. Simulation of Plectonemic Supercoil Diffusion Along Extended DNA. Proceedings 56th Annual Meeting, Biophysical Society, San Diego, California. Poster.