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I. Profession

2017.05 - now	**Associate Professor** of Physics (Tenured), George Washington University
2015.04 - 2023.04	**Founding Co-Director**, GW Center for BioMolecular Sciences (GWCBMS)
2013.09 - 2016.09	Member of the International Relations Committee, Biophysical Society
2010.08 - 2017.05	**Assistant Professor** of Physics (Tenure-Track), George Washington University
2007.06 - 2010.06	**Research Fellow**, Physical & Structural Biology Lab, National Institutes of Health

II. Education & Training

2004.09 - 2007.06	**Postdoctoral Associate** in Experimental Biophysics, Cornell University Supervisor: Dr. Lois Pollack
1999.09 - 2004.08	**Ph.D.** in Experimental Condensed Matter Physics, Michigan State University, USA Supervisor: Dr. Simon J. L. Billinge
1994.09 - 1999.07	**B.S.** in Physics & **B.E.** in Computer Science, Univ. of Science & Technology of China

III. Research Activities

III.1 Current Interests

1. **Physics-inspired neural networks for predictive nucleic acids biology**. Building on the rapid progress in nucleic acids big data and artificial intelligence algorithms, we develop biophysics-inspired neural networks to codify and predict nucleic acids structure, function, and evolution dynamics.
2. **Exploration of new data dimensions of nucleic acids structural biology**. Using both wet-lab experiments, bioinformatics, and simulations, we examine the often-ignored sequence-dependent molecular mechanics of nucleic acids and the small-molecule environments as new information dimensions for both mechanistic understanding and machine learning.
3. **Nucleic acids drug design and gene delivery**. Inspired by the revolutionary potential and modern advances of genetic medicine, we strive to translate our computational and experimental expertise in nucleic acids research into the design of nucleic acids sequences for therapeutic purposes and the development of targeted gene delivery mechanisms.

III.2 Software Tools

1. **SeqFold2D**: A deep learning model to predict RNA secondary structures from single sequences.

   Code: *https://github.com/qiuresearch/SeqFold2D*
   Article:
   Sequence similarity governs generalizability of de novo deep learning models for RNA secondary structure prediction, PLoS Comput Biol 19(4): e1011047, 2023.

2. **RNA-UPP**: A deep learning model to predict the unpaired probabilities of RNA from single sequences. **Ranked No. 1** out of 1000+ players, Baidu AI Contest for RNA Structure Prediction, 2021/05
(as the sole member of the team titled Genetic Therapy, *contest website on Baidu AIstudio*)

   Code: *https://github.com/genetic-medicine/PaddleHelix_RNA_UPP*

   Article:
   Deep learning algorithms for RNA Structure Prediction: part I
   Deep learning algorithms for RNA Structure Prediction: part II

3. **MatLib**: Various programs and scripts for data analysis and modelling in experimental biophysics research. Main functions include 1) AtomSAXS, a script to calculate solution small angle x-ray scattering (SAXS) profiles of atomistic models of biomolecules, 2) XYpro, a GUI-driven program for visualizing and curve-fitting of one-dimensional data, and 3) SQfit, a GUI-driven program for fitting inter-particle interference patterns to obtain inter-particle potentials.

   Code: *https://github.com/qiuresearch/matlib*

III.3 All Peer-reviewed Articles ($^{\#}$: corresponding author; $^{\bigstar}$: supervised student/postdoc)

Since Joining GW, August 2010 – now

1. W. He, **X. Qiu**$^{\#}$, S. Kirmizialtin$^{\#}$, *Sequence-dependent orientational coupling and electrostatic attraction in cation-mediated DNA-DNA interactions*, **Journal of Chemical Theory and Computation**, in press (2023). **[Cover Article]**

2. **X. Qiu**$^{\#}$, *Sequence similarity governs generalizability of de novo deep learning models for RNA secondary structure prediction.* , **PLoS Comput Biol** , 19(4): e1011047 (2023).

3. B. Kopchick$^{\bigstar\#}$, H. Xu, Y. Niu, S. Becker, **X. Qiu**, and C. Yu, *Dosimetric feasibility of lattice radiotherapy for breast cancer using GammaPod*, **Medical Physics**, 48(13), 7018–7026 (2020).

4. W. Meng$^{\bigstar}$, R. Timsina$^{\bigstar}$, A. Bull, K. Andresen$^{\#}$, and **X. Qiu**$^{\#}$, *Additive Modulation of DNA-DNA Interactions by Interstitial Ions*, **Biophysical Journal**, 118, 1–7 (2020).

5. A. Srivastava, R. Timsina$^{\bigstar}$, S. Heo$^{\bigstar}$, S. W. Dewage, S. Kirmizialtin$^{\#}$, and **X. Qiu**$^{\#}$, *Structure-guided DNA–DNA attraction mediated by divalent cations*, **Nucleic Acids Research**, 48(13), 7018–7026 (2020).

6. S-J. Lee, D. Asheghali, B. Blevin, R. Timsina$^{\bigstar}$, T. Esworthy, X. Zhou, H. Cui, S. Y. Hann, **X. Qiu**, A. Tokarev, S. Minko, and L. G. Zhang$^{\#}$, *Touch-Spun Nanofibers for Nerve Regeneration*, **ACS Applied Materials & Interfaces** , 12, 2067-2-075 (2020).

7. D. N. Heo, S-J. Lee, R. Timsina$^{\bigstar}$, **X. Qiu**, N. J. Castro, and L. G. Zhang$^{\#}$, *Development of 3D printable conductive hydrogel for enhancing neuronal cell differentiation*, **Materials Science and Engineering: C**, 99, 582–590 (2019).

8. W. Zhang, S. C. Howell$^{\bigstar}$, D. W. Wright, A. Heindeld, **X. Qiu**, J. Chen$^{\#}$, and J. E. Curtis$^{\#}$, *Combined Monte Carlo/torsion-angle molecular dynamics for ensemble modeling of proteins, nucleic acids and carbohydrates*, **Journal of Molecular Graphics and Modeling**, 73, 179–190 (2017).

9. S. .C. Howell★#, **X. Qiu**, and J. Curtis, *Monte Carlo Modelling of dsDNA for Small Angle Scattering*, **Journal of Computational Chemistry**, 37 (29), 2553–2563 (2016). **[Journal Cover Article]**

10. **X. Qiu**#, F. Ke★, R. Timsina★, C. Y. Khripin, and M. Zheng, *Attractive Interactions between DNA-Carbon-Nanotube Hybrids in Monovalent Salts*, **Journal of Physical Chemistry C**, 120 (25), 13831–13835 (2016).

11. W. Meng★, E. Gall★, F. Ke★, Z. Zeng★, and **X. Qiu**#, *Structure and Interaction of Graphene Oxide-CTAB Complexation*, **Journal of Physical Chemistry C**, 119 (36), 21135–21140 (2015).

12. F. Ke★, and **X. Qiu**#, *Nanoscale Structure and Interaction of condensed phases of DNA-Carbon Nanotube Hybrids*, **Journal of Physical Chemistry C**, 119 (27), 15763–15769 (2015).

13. D. Li, T. Liu, X. Zuo, T. Liu, **X. Qiu**, and A. Evilevitch#, *Not Only a Genetic Switch but also an Ionic Switch Controls Phage λ Replication*, **Nucleic Acids Research**, 43 (13), 6348-6358 (2015).

14. J. Li, S. S. Wijeratne, **X. Qiu**#, and C.-H. Kiang#, *DNA under Force: Mechanics, Electrostatics, and Hydration*, **Nanomaterials**, **5(1)**, 246-267 (2015).

15. J. Zhou, H. Wen, F. Ke★, D. Shi, A. A. Brisky★, N. Wang, L. Zhu, **X. Qiu**#, and D. Liang#, *Capsules with a hierarchical shell structure assembled by aminoglycosides and DNA via the kinetic path*, **Chemical Communications**, **50**(67), 9525-9528 (2014).

16. K. Andresen#, I. Jimenez-Useche, S. C. Howell★, C. Yuan, and **X. Qiu**#, *Local and global structure determination of DNA unwrapping of the nucleosome* , **PLoS One**, **8**(11), e78587 (2013).

17. **X. Qiu**#, J. Giannini, S. C. Howell★, Q. Xia★, F. Ke★, and K. Andresen#, *Ion Competition in Condensed DNA Arrays in the Attractive Regime*, **Biophysical Journal**, **105**(4), 984–992 (2013).

18. I. Jimenez-Useche, J. Ke★, Y. Tian, D. Shim, S. C. Howell★, and **X. Qiu**, and C. Yuan#, *DNA Methylation Regulated Nucleosome Dynamics*, **Scientific Reports**, **3**, 2121 (2013).

19. **X. Qiu**#, C. Khripin, F. Ke★, S. C. Howell★, and M. Zheng , *Electrostatics-driven Interactions between Hybrids of DNA-Carbon Nanotubes*, **Physical Review Letters**, **111**(4), 048301 (2013).

20. S. C. Howell★, K. Andresen, I. Jimenez-Useche, C. Yuan, and **X. Qiu**#, *Measuring inter-nucleosome interactions and the roles of histone tails*, **Biophysical Journal**, **105**, 194–199 (2013).

21. **X. Qiu**#, *Heat-induced capsid disassembly and DNA release of bacteriophage λ*, **PLoS One**, **7(7)**, e39793 (2012).

22. **X. Qiu**#, D. C. Rau, V. A. Parsegian, L. T. Fang, C. M. Knobler, and W. M. Gelbart, *Salt-dependent DNA-DNA spacings in intact bacteriophage lambda reflect relative importance of DNA self-repulsion and bending energies*, **Physical Review Letters**, **106**, 028102 (2011).

23. **X. Qiu**#, V. A. Parsegian, and D. C. Rau, *Divalent counterion induced condensation of triple-strand DNA*, **Proceedings of the National Academy of Sciences**, **107** (50), 21482–21486 (2010).

Postdoctoral Research at Cornell and NIH, September 2004 – June 2010

24. **X. Qiu**#, and P. Setlow#, *Structural and genetic analysis of x-ray scattering of bacterial spores*, **Journal of Bacteriology**, **191** (24), 7620 (2009).

25. S. A. Pabit, **X. Qiu**, J. S. Lamb, L. Li, S. P. Meisburger, and L. Pollack#, *Counterions more effectively screen dsRNA than dsDNA*, **Nucleic Acids Research**, **37** (12), 3887 (2009).

26. J. S. Lamb, L. W. Kwok, **X. Qiu**, K. Andresen, H.-Y. Park, and L. Pollack#, *Reconstructing three dimensional shape envelopes from time resolved small angle x-ray scattering data*, **Journal of Applied Crystallography**, **41**, 1046–1052 (2008).

27. **X. Qiu**, K. Andresen, J. S. Lamb, L. W. Kwok, and L. Pollack#, *Abrupt transition from free, repulsive to condensed, attractive DNA phase, induced by multivalent polyamine cations*, **Physical Review Letters**, **101**, 228101 (2008).

28. K. Andresen, **X. Qiu**, J. S. Lamb, H.-Y. Park, L. W. Kwok, and L. Pollack#, *Mono- and Tri-valent Ions around DNA: A Small-Angle Scattering Study of Competition and Interactions*, **Biophysical Journal**, **95**, 287–295 (2008).

29. **X. Qiu**, K. Andresen, L. W. Kwok, J. S. Lamb, H.-Y. Park, and L. Pollack#, *Inter-DNA attraction mediated by divalent counterions*, **Physical Review Letters**, **99**, 038104 (2007).

30. J. S. Lamb, S. Cornaby, K. Andresen, L. Kwok, H.-Y. Park, **X. Qiu**, D. M. Smilges, D. H. Bilderback, and L. Pollack#, *Focusing capillary optics for use in SAXS*, **Journal of Applied Crystallography**, **40**, 193–195 (2007).

31. **X. Qiu**, L. W. Kwok, H.-Y. Park, J. S. Lamb, K. Andresen, and L. Pollack#, *Measuring Inter-DNA Potentials in Solution*, **Physical Review Letters**, **96**, 138101 (2006).

32. H.-Y. Park, **X. Qiu**, E. Rhoades, J. Korlach, L. W. Kwok, W. R. Zipfel, W. W. Webb, and L. Pollack#, *Achieving uniform mixing in a microfluidic device: hydrodynamic focusing prior to mixing*, **Analytical Chemistry**, **78** (13), 4465–4473 (2006).

PhD Thesis Research at Michigan State, September 2000 – August 2004

33. G. Campi, Th. Proffen, **X. Qiu**, E. S. Božin, S. J. L. Billinge, S. Agrestini, N.L. Saini, and A. Bianconi#, *Local lattice dynamics in the $Mg_{0.5}Al_{0.5}B_2$ superconductor*, **Journal of Superconductivity and Novel Magnetism**, **20**, 505–510 (2007).

34. E. Božin, **X. Qiu**, R. J. Worhatch, G. Paglia, M. Schmidt, P. G. Radaelli, J. F. Mitchell, T. Chatterji, Th. Proffen, and S. J. L. Billinge#, *Utilizing total scattering to study the Jahn-Teller transition in $La_{1-x}Ca_xMnO_3$*, **Z. Kristallography**, Suppl. **26**, 429–434 (2007).

35. G. Campi, E. Cappelluti, Th. Proffen, **X. Qiu**, E. S. Božin, S. J. L. Billinge, S. Agrestini, N.L. Saini, and A. Bianconi#, *Study of temperature dependent atomic correlations in MgB_2*, **The European Physical Journal B**, **52**, 15–21 (2006).

36. E. S. Božin, **X. Qiu**, M. Schmidt, G. Paglia, J. F. Mitchell, P. G. Radaelli, Th. Proffen, and S. J. L. Billinge#, *Local structural aspects of the orthorhombic to pseudo-cubic phase transformation in $La_{1-x}Ca_xMnO_3$*, **Physica B**, (385–386), 110–112 (2006).

37. **X. Qiu**, Th. Proffen, J. F. Mitchell, and S. J. L. Billinge#, *Orbital correlations in the pseudo-cubic* O *and rhombohedral* R*-phases of $LaMnO_3$*, **Physical Review Letters**, **94**, 177203 (2005).

38. **X. Qiu**, J. W. Thompson, and S. J. L. Billinge[#], *PDFgetX2: A GUI driven program to obtain the pair distribution function from x-ray powder diffraction data*, **Journal of Applied Crystallography**, **37**, 678 (2004).

39. **X. Qiu**, S. J. L. Billinge[#], C. R. Kmety, and J. F. Mitchell[#], *Evidence for nano-scale inhomogeneities in bilayer manganites in the Mn^{4+} rich region: $0.54 \leq x \leq 0.80$*, **Journal of Physics and Chemistry of Solids**, **65**, 1423–1429 (2004).

40. P. J. Chupas, S. Chaudhuri, J. C. Hanson, **X. Qiu**, P. L. Lee, S. D. Shastri, S. J. L. Billinge and C. P. Grey[#], *Simultaneous local and long range structure determination: application to in-situ studies of the high temperature phase transition of α-AlF_3*, **Journal of the American Chemical Society**, **126**, 4756–4757 (2004).

41. **X. Qiu**, E. S. Bozin, P. Juhas, Th. Proffen, and S. J. L. Billinge[#], *Reciprocal-space instrumental effects on the real-space neutron atomic pair distribution function*, **Journal of Applied Crystallography**, **37**, 110–116 (2004).

42. S. Derakhshan, A. Assoud, E. Dashjav, **X. Qiu**, S. J. L. Billinge, and H. Kleinke[#], *Distorted nets of Ti atoms comprising squares and rhombs in the new binary antimonide Ti_2Sb*, **Journal of the American Chemical Society**, **126**, 8295–8302 (2004).

43. P. J. Chupas, **X. Qiu**, J. C. Hanson, P. L. Lee, C. P. Grey, and S. J. L. Billinge[#], *Rapid-acquisition pair distribution function (RA-PDF) analysis*, **Journal of Applied Crystallography**, **36**, 1342–1347 (2003).