CURRICULUM VITAE

Name

Margaret Shun Cheung
Physicist, UW-PNNL Faculty Fellow of Physics
Pacific Northwest National Laboratory
University of Washington, Seattle
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Education

National Taiwan University	B.Sci. Chemistry	June, 1994
University of California at San Diego	Ph.D. Physics	March, 2003
University of Maryland	Sloan Postdoctoral Fellow	May, 2003- August, 2006

Employment

Physicist, Pacific Northwest National Laboratory 2021-present
Earth and Biological Sciences Directorate

UW-PNNL Faculty Fellow, University of Washington, Seattle 2021-present
Department of Physics

Adjunct Professor, Rice University 2018-2022
Department of Bioengineering

Senior Scientist, Rice University 2012-2022
Center for Theoretical Biological Physics

Moores Professor, University of Houston 2018-2022

Professor, University of Houston 2017-2022
Department of Physics
Department of Chemistry (courtesy appointment)
Department of Computer Science (courtesy appointment)

Associate Professor, University of Houston 2012-2017
Department of Physics

Assistant Professor, University of Houston 2006-2012
Department of Physics

Sloan Postdoctoral Fellow, University of Maryland, College Park 2003- 2006
Institute for Physical Science and Technology,
Research advisor: Prof. Devarajan Thirumalai,
Effects of crowding and confinement on protein-protein interaction

Graduate Researcher, University of California, San Diego 1997- 2003
Department of Physics/Center for Theoretical Biological Physics
Thesis advisor: Prof. José N. Onuchic,
Energy landscape aspect of protein folding dynamics relevant to molecular functions

Fellowship and Awards

2023 – PNNL Exceptional Contribution Award
2022 – UW Louise Stokes Alliance for Minority Participation (LSAMP) Faculty of the Year Award
2019 – Robert S. Hyer Research Award
2018 – Moores Professorship
2016 – UH Excellence in Research and Scholarship (Associate Professor)
2013 – Fellow of the American Physical Society
2012 – UH Excellence in Research and Scholarship (Assistant Professor)
2010 – Robert S. Hyer Research Award
2006 – University of Houston New Faculty Award
2003-2006 Alfred P. Sloan Foundation Postdoctoral Fellowship
1990-1991 National Taiwan University Book Coupon Award

Research Interests

- Emergent protein assemblies in a cell
- Imaging and integrative modeling of biomolecular assemblies
- Organization of protein-mediated actomyosin networks
- Regulatory protein structures in metabolic networks
- Molecular biophysics in calmodulin-mediated calcium signaling network
- Molecular design of biomimetic materials for switchable functions

Ongoing Research Support

Active

Enhancing Biopreparedness through a Model System to Understand the Molecular Mechanisms that Lead to Pathogenesis and Disease Transmission
Department of Energy, Biological and Environmental Research (81832), $10,800,000
Role: PI Cheung
Organization: Pacific Northwest National Laboratory
Duration: 09/01/23-08/31/26

Emergent Protein Assemblies in Cytoplasm
National Science Foundation (MCB 2221824), $813,012
Role: PI
Organization: University of Washington
Duration: 08/01/22 - 07/31/26

Predicting cellular states from emergent protein assemblies
PNNL Laboratory Directed Research and Development (79581), $738,000
Role: PI
Organization: Pacific Northwest National Laboratory
Duration: 03/01/22-09/30/24

Joint Appointment – UW
University of Washington, $6000

Role: PI
Organization: University of Washington
Duration: 01/01/22-02/29/24

Manipulating Signaling Proteins for Target Binding and Recognition
National Institutes of Health (2R01GM097553), $1,131,944
Role: PI
Organization: University of Washington (transferred from University of Houston)
Duration: 06/01/16 - 04/30/23

Recently Completed Research Support

Virtual Proteomics: Integrative Modeling of Protein Assemblies in a Cell from High-throughput Proteomic Data and Reconstructed Cryotomography Images
PNNL Laboratory Directed Research and Development (78215), $300,000
Role: PI
Organization: Pacific Northwest National Laboratory
Duration: 03/2021 – 09/2022

Accurately Predict the Spatial Arrangement of Protein Complexes from Subtomogram Images through Physics-informed Machine Learning
DOE Biological and Environmental Research (77756), $256,887
Role: PI
Organization: Pacific Northwest National Laboratory
Duration: 11/2021-10/2023

RAISE: Dendritic Spine Mechano-Biology and the Process of Memory Formation (PI: Peter Wolynes at Rice)
National Science Foundation (CHE-1743392), $996,778
Role: Co-PI
Organization: Rice University
Duration: 08/15/17- 07/31/23 (No-cost extension)

Center for Theoretical Biological Physics (PI: Jose' Onuchic at Rice)
National Science Foundation (PHY2019745), Subcontract from Rice to UH: $751,771
Role: PI at UH
Duration: 09/01/20- 07/01/22

Post-Marcus Theory and Simulation of Interfacial Charge Transfer Dynamics in Organic Semiconducting Materials (PI: Barry Dunietz at Kent State)
Department of Energy (DE-SC0016501), subcontract from Kent State to UH, $300,000
Role: PI at UH
Duration: 09/15/17-09/14/21 (No cost extension)

Journal Publications (in reverse chronological order)

Original Research Articles

76. X. Li, X. Yin, N. Wiebe, J. Chun, G. K. Schenter, M. S. Cheung, J. Muelmenstaedt, "Potential quantum advantage for simulation of fluid dynamics", https://arxiv.org/abs/2303.16550 *submitted* (2023).

75. C. Li, T. Wei, M.S. Cheung, M.Y. Tsai, "Deciphering the cofilin oligomers via intermolecular disulfide bond formation: A coarse-grained molecular dynamics approach to understanding cofilin's regulation on actin filament", *submitted* (2023).

74. D. Mejia-Rodriguez*, H. Kim*, N. Sadler, X. Li, P. Bohutskyi, M. Valiev, W.-J. Qian, M. S. Cheung, "PTM-Psi: A python package to facilitate the computational investigation of post-translational modification on protein structures and their impacts on dynamics and functions", accepted by *Protein Science* (2023).

73. J. Nde, P. Zhang, M. N. Waxham, M. S. Cheung, "Experiment and simulation reveal residue details for how polymorphous target binding tunes calmodulin's calcium-binding properties", *J. Phys. Chem. B, 127,* 2900-2908 (2023).

72. A. George, D. N. Kim, T. Moser, I. T. Gildea, J. Evans, M. S. Cheung, "Graph identification of proteins in tomographs (GRIP-Tomo)", *Protein Science, 32*, e4538 (2023).

71. A. Sarkar, A. G. Gasic, M. S. Cheung, G. C. Morrison, "Effects of protein crowders and charge on the folding of superoxide dismutase 1 variants: a computational study", *J. Phys. Chem. B. 126,* 4458-4471(2022).

70. C. Bueno, J. Liman, N. P. Schafer, M. S. Cheung, P. G. Wolynes, "A generalized Flory-Stockmayer kinetic theory of connectivity percolation and rigidity percolation of cytoskeletal network", *PoLS Comp. Biol. 18,* e1010105 (2022).

69. J. Tinnin, S. Bhandari, P. Zhang, E. Geva, B. D. Dunietz, X. Sun, M. S. Cheung, "Correlating interfacial charge transfer rates with interfacial molecular structure in the tetraphenyldibenzoperiflanthene/C70 organic photovoltaic system", *J. Phys. Chem. Lett., 13,* 763-769 (2022).

68. C. Li, J. Liman, Y. Eliaz, M. S. Cheung, "Forecasting avalanches in branched actomyosin networks with network science and machine learning", *J. Phys. Chem. B, 125,* 11591-11605 (2021).

67. J. Nde, P. Zhang, J. C. Ezerski, P. G. Wolynes, M. S. Cheung, "Coarse-grained modeling and molecular dynamics simulations of Ca^{2+}-calmodulin", *Frontiers in Molecular Sciences, 8,* 661322 (2021).

66. A. G. Gasic, A. Sharkar, M. S. Cheung, "Understanding protein complex assembly through grand canonical maximum entropy modeling", *Physical Rev. Research, 3,* 033220 (2021).

65. J. Tinnin, S. Bhandari, P. Zhang, H. Aksu, B. Maiti, E. Geva, B. D. Dunietz, X. Sun, M. S. Cheung, "CTRAMER: software for calculating charge-transfer-rate constants with condensed-phase effects", *J. Chem. Phys. 154,* 214108 (*2021*).

64. F. C. Zegarra, D. Homouz, P. Wittung-Stafshede, M. S. Cheung, "The zero-order loop in apoazurin modulates unfolding in silico", *J. Phys. Chem. B, 125*, 3501-3509 *(2021).*

63. P. Zhang, J. Han, P. Cieplak, M. S. Cheung, "Determining the atomic charge of calcium ion in a calcium-binding protein requires the information of its dynamic coordination geometry in aqueous solution", *J. Chem. Phys. 154,* 124104 (2021).

62. Y. Eliaz, F. Nedelec, G. Morrison, H. Levine, M. S. Cheung, "Multivalent actin-binding proteins augment the variety of morphologies in actomyosin networks", *Phys. Rev. E 102,* 062420 (2020).

61. J. Han, P. Zhang, H. Aksu, B. Maiti, X. Sun, E. Geva, B. Dunietz, M. S. Cheung, "On the interplay between electronic structure and polarizable force fields when calculating solution-phase charge-transfer rates", *J. Chem. Theory Comput. 16,* 6481–6490 (2020).

60. Z. Hu, Z. Tong, M. S. Cheung, B. Dunietz, E. Geva, X. Sun, "Photoinduced charge transfer dynamics in carotenoid-porphyrin-C_{60} triad via the linearized semiclassical nonequilibrium Fermi's golden rule", *J. Phys. Chem. B, 124,* 9579–9591 (2020).

59. Z. Tong, X. Gao, M. S. Cheung, B. Dunietz, E. Geva, X. Sun, "Charge transfer rate constants for the carotenoid-porphyrin-C_{60} molecular triad dissolved in tetrahydrofuran: the spin-boson model vs. the linearized semiclassical approximation", *J. Chem. Phys. 153,* 044105 (2020).

58. J. Tinnin, S. Bhandari, P. Zhang, H. Aksu, B. Maiti, E. Geva, B. D. Dunietz, X. Sun, M. S. Cheung, "Molecular-level exploration of the structure-function relations underlying interfacial charge transfer in the subphthalocyanine:C_{60} organic photovoltaic system", *Phys. Rev. Applied, 13,* 054075 (2020).

57. J. Liman, C. Bueno, Y. Eliaz, M. N. Waxham, H. Levine, P. G. Wolynes, M. S. Cheung, "The contractility of actomyosin network in the presence of arp2/3", *Proc. Natl. Acad. Sci. 117,* 10825-10831 (2020).

56. J. C. Ezerski, P. Zhang, N. C. Jennings, M. N. Waxham, M. S. Cheung, "Molecular dynamics ensemble refinement of intrinsically disordered peptides from circular dichroism spectra", *Biophys. J*, *118*, 1665-1678 (2020).

55. A. G. Gasic, M. S. Cheung, "A tale of two desolvation potentials: an investigation of protein behavior under high hydrostatic pressure", *J. Phys. Chem. B, 124,* 1619-1627 (2020).

54. K. Dave, A. G. Gasic, M. S. Cheung, M. Gruebele, "Competition of folding and inter-domain

aggregation in tethered WW domains", *Phys. Chem. Chem. Phys., 21,* 24393-24405 (2019).

53. A. G. Gasic, M. M. Boob, M. B. Prigozhin D. Homouz, C. M. Daugherty, M. Gruebele, M. S. Cheung, "Critical phenomena in the temperature-pressure-crowding phase diagram of a protein", *Phys. Rev. X, 9,* 041035 (2019).

52. Q. Wang, M. Chen, C. Bueno, S. S. Song, A. Hudman, M. N. Waxham, P. G. Wolynes, M. S. Cheung, "Calcium/Calmodulin dependent kinase II – actin assemblies and their dynamic regulation by calmodulin in dendritic spines", *Proc. Natl. Acad. Sci., 116,* 18937-18942 (2019).

51. M. Ghane, M. S. Cheung, S. Chandrasekaran, "Pointerchain: Tracing pointers to their root", *Parallel Computing*, *85*, 190-203 (2019).

50. F. C. Zegarra, D. Homouz, M. Kovermann, A. G. Gasic, L. Babel, P. Wittung-Stafshede, M. S. Cheung, "Crowding-induced elongated conformation of urea-unfolded apoazurin explained by *in silico* computations: Key role of crowder shape", *J. Phys. Chem. B*, *123*, 3607–3617 (2019).

49 J. C. Ezerski, M. S. Cheung, "CATS: a tool for clustering the ensemble of intrinsically disordered peptides on a flat energy landscape", *J. Phys. Chem. B*, *122*, 11807–11816 (2018).

48. S. Bhandari, M. S. Cheung, E. Geva, L. Kronik, B. D. Dunietz, "Fundamental gaps of condensed-phase organic semiconductors from single-molecule calculations using polarizable consistent optimally tuned screened range-separated hybrid functionals", *J. Chem. Theory Comput.*, *14*, 6287-6294 (2018).

47. Q. Wang, B. Janab, M. R. Diehl, M. S. Cheung, A. B. Kolomeisky, J. N. Onuchic, "Molecular mechanisms of the interhead coordination by interhead tension in cytoplasmic dyneins", *Proc. Natl. Acad. Sci. U.S.A., 115,* 10052-10057 (2018).

46. X. Sun, P. Zhang, Y. Lai, K. Williams, M. S. Cheung, B. Dunietz, E. Geva, "A computational study of charge transfer dynamics in the carotenoid porphyrin C60 molecular triad solvated in explicit tetrahydrofuran and its spectroscopic signature", *J. Phys. Chem. C*, *122*, 11288–11299 (2018).

45. M. Misiura, Q. Wang, M. S. Cheung, A. B. Kolomeisky, "Theoretical investigation of the role of mutation in dynamics of kinesin motor protein", *J. Phys. Chem. B, 122*, 4653-4661 (2018).

44. F. C. Zegarra, D. Homouz, Y. Eliaz, A. G. Gasic, M. S. Cheung, "The impact of hydrodynamic interactions on protein folding rates depends on temperature", *Phys. Rev. E, 97*, 032402 (2018).

43. Q. Wang, M. R. Diehl, B. Jana, M. S. Cheung, A. B. Kolomeisky, J. N. Onuchic, "Molecular origin of the weak susceptibility of kinesin velocity to loads and its relation to the collective behavior of kinesins", *Proc. Natl. Acad. Sci. U. S. A.*, *114*, E8611-E8617 (2017).

42. O.N. Starovoytov, P. Zhang, P. Cieplak, , M. S. Cheung, "Induced polarization restricts conformational distribution of a light-harvesting molecular triad in the ground state", *Phys. Chem. Chem. Phys.*, *19*, 22969-22980 (2017).

41. P. Zhang, L. S. Tripathi, H. Trinh, M. S. Cheung, "Opposing intermolecular tuning of Ca2+ affinity for calmoduin by target peptide", *Biophys. J., 112*, 1105–1119 (2017).

40. M.Y. Tsai, W. Zheng, D. Balamurugan, N.P. Schafer, B.L. Kim, M.S. Cheung, P.G. Wolynes, "Electrostatics, structure prediction and the energy landscapes for protein folding and binding", *Protein Science, 25*, 255-269 (2016).

39. S. Tripathi, L. Belkacemi, M. S. Cheung, R. N. Bose, "Correlation between gene variants, signaling pathways and efficacy of chemotherapy drugs against colon cancers", *Cancer Informatics*, *15*, 1-13 (2016).

38. L. Hoffman, X. Wang, H. Sanabria, M. S. Cheung, J. Putkey, M. N. Waxham, "Tuning of protein function by macromolecular crowding", *Biophys. J.*, *109*, 510-520 (2015).

37. S. Tripathi, M. N. Waxham, M. S. Cheung, Y. Liu, "Lessons in Protein Design from Combined Evolution and Conformational Dynamics", *Scientific Reports, 5*, 14259 (2015).

36. A. K. Manna, D. Balamurugan, M. S. Cheung, B. D. Dunietz, "Unraveling the mechanism of photo-induced charge-transfer in carotenoid-porphyrin-C60 molecular triad", *J. Phys. Chem. Lett., 6*, 1231-1237 (2015).

35. S. Tripathi, P. Zhang, Q. Wang, L. Hoffman, M. N. Waxham, M. S. Cheung, "Conformational Frustration in Calmodulin-Target Recognition", *Journal of Molecular Recognition, 28*, 74–86 (2015)

34. Q. Wang, P. Zhang, S. Tripathi, L. Hoffman, L. Yin, M. N. Waxham, M. S. Cheung, "Protein recognition and selection through conformational and mutually induced fit", *Proc. Natl. Acad. Sci. U. S. A.*, *110*, 20545-20550 (2013).

33. D. Balamurugan, A. J. A. Aquino, F. De Dios, L. Flores Jr., H. Lischka, M. S. Cheung, "Multiscale simulation of the ground and photo-induced charge-separated states of molecular triad in polar organic solvent: exploring the conformations, fluctuations and the free energy landscapes", *J. Phys. Chem. B., 117*, 12065-12075 (2013).

32. E. Chen, A. Christiansen, Q. Wang, M. S. Cheung, D.S. Kliger, P. Wittung-Stafshede, "Crowd control and the effects of macromolecular crowding on burst phase kinetics of cytochrome c folding", *Biochemistry*, *51*, 9836-9845 (2012).

31. A. Kudlay, M. S. Cheung, D. Thirumalai, "Influence of the Shape of Crowding Particles on the Structural Transitions in a Polymer", *J. Phys. Chem. B, 116*, 8513–8522 (2012).

30. Q. Wang, M. S. Cheung, "A Physics-based approach of coarse-graining the cytoplasm of *E. coli* (CGCYTO)", *Biophys. J., 102*, 2353-2361 (2012).

29. G. Su, A. Czader, D. Homouz, G. Bernardes, S. Mateen, M. S. Cheung, "Multiscale simulation on a light-harvesting molecular triad", *J. Phys. Chem. B, 116,* 8460–8473 (2012).

28. Q. Wang, A. Christiansen, A. Samiotakis, P. Wittung-Stafshede, M. S. Cheung, "Part II. Comparison of chemical and thermal protein denaturation by combination of computational and experimental approaches", *J. Chem. Phys.*, *135*, 175102 (2011).

27. A. Samiotakis, M. S. Cheung, "Part I. Folding dynamics of Trp-cage in the presence of chemical interference and macromolecular crowding", *J. Chem. Phys.*, *135*, 175101 (2011).

26. Q. Wang, K.-C. Liang, A. Czader, M. N. Waxham, M. S. Cheung, "The effect of macromolecular crowding, ionic strength and calcium binding on calmodulin dynamics", *PLoS Comp. Biol., 7,* e1002114 (2011).

25. Q. Wang, G. Hong, J. Glenn, R. Pachter, M. S. Cheung, "Biophysical properties of membrane-active peptides based on micelle modeling: A case study of cell-penetrating and antimicrobial peptides", *J. Phys. Chem. B, 114*, 13726-13735 (2010).

24. A. Dhar, A. Samiotakis, S. Ebbinghaus, L. Nienhaus, D. Homouz, M. Gruebele, M. S. Cheung, "Structure, function and folding of phosphoglycerate kinase are strongly perturbed by macromolecular crowding", *Proc. Natl. Acad. Sci. U. S. A., 107*, 17586-17591 (2010).
    - *Commentary "Crowding and Function Reunite" by G. J. Pielak and A. C. Miklos, PNAS, 107, 17457-17458 (2010).*

23. A. Christiansen, Q. Wang, A. Samiotakis, M. S. Cheung, P. Wittung-Stafshede, "Factors defining effects of macromolecular crowding on protein stability: an *in vitro/in silico* case study using cytochrome c", *Biochemistry, 49*, 6519-6530 (2010).

22. A. Samiotakis, D. Homouz, M. S. Cheung, "Multiscale investigation of chemical interference in proteins", *J. Chem. Phys., 132,* 175101 (2010).

21. L. Stagg, A. Samiotakis, M. S. Cheung, P. Wittung-Stafshede, "Residue specific analysis of frustration in folding landscape of repeat β/α protein apoflavodoxin", *J. Mol. Biol., 396*, 75-89 (2010).

20. D. Homouz, H. Sanabria, M. N. Waxham, M. S. Cheung, "Modulation of calmodulin plasticity by the effect of macromolecular crowding", *J. Mol. Biol., 391*, 933-943 (2009).

19. D. Homouz, B. Hoffman, M. S. Cheung, "Hydrophobic interactions of hexane in nanosized water droplets", *J. Phys. Chem. B, 113*, 12337-12342 (2009).

18. A. Kudlay, M. S. Cheung, D. Thirumalai, "Crowding effects on the structural transitions in a flexible helical homopolymer", *Phys. Rev. Letts., 102*, 118101 (2009).

17. D. Homouz, L. Stagg, P. Wittung-Stafshede, M. S. Cheung, "Macromolecular crowding modulates folding mechanism of α/β protein apoflavodoxin", *Biophys. J., 96*, 671-680 (2009).

16. D. Homouz, M. Perham, A. Samiotakis, M. S. Cheung, P. Wittung-Stafshede. "Crowded, cell-like environment induces shape changes in aspherical protein", *Proc. Natl. Acad. Sci. U. S. A., 105,* 11754-11759 (2008).
    - *Featured as best biophysics paper in Research Highlights of 2008 in Nature.*

15. L. Stagg, S.-Q. Zhang, M. S. Cheung, P. Wittung-Stafshede, "Molecular crowding enhances native structure and stability of α/β protein flavodoxin", *Proc. Natl. Acad. Sci. U. S. A., 104,* 18976-18981 (2007).

14. S.-Q. Zhang, M. S. Cheung, "Manipulating Biopolymer Dynamics by Anisotropic Nanoconfinement", *Nano Letters, 7,* 3438-3442 (2007).

13. M. S. Cheung, D. Thirumalai, "Crowding and confinement effects on structures of the transition state ensemble in proteins", *J. Phys. Chem. B, 111*, 8250-8257 (2007).

12. M. E. Sardiu, M. S. Cheung, Y.-K. Yu, "Cysteine-Cysteine contact preference leads to target-focusing in protein folding", *Biophys., J., 93*, 1-14 (2007).

11. M. S. Cheung, D. Thirumalai, "Nanopore-protein interactions dramatically alter stability and yield of the native state in restricted spaces", *J. Mol. Biol., 357*, 632-643 (2006).

10. J. Chahine, M. S. Cheung, "Computational studies of the reversible domain swapping of p13suc1", *Biophys. J., 89,* 1-9 (2005).

9. M. S. Cheung, D. Klimov, D. Thirumalai, "Molecular crowding enhances native state stability and refolding rates", *Proc. Natl. Acad. Sci. U. S. A., 102*, 4753-4758 (2005).

8. S. Yang, S. S. Cho, Y. Levy, M. S. Cheung, H. Levine, P. G. Wolynes, J. N. Onuchic, "Domain swapping is a consequence of minimal frustration", *Proc. Natl. Acad. Sci. U. S. A., 101*, 13786-13791 (2004).

7. J. M. Finke, M. S. Cheung, J. N. Onuchic, "A structural model of polyglutamine determined from a host-guest method combining experiments and landscape theory", *Biophys. J.*, *87,* 1900-1918 (2004).

6. A. Fernandez-Escamilla, M. S. Cheung, M. C. Vega, M. Wilmanns, J. N. Onuchic, L. Serrano, "Solvation in protein folding analysis, combination of theoretical and experimental approaches", *Proc. Natl. Acad. Sci. U. S. A., 101,* 2834-2839 (2004).

5. M. S. Cheung, L. L. Chavez, J. N. Onuchic, "The Energy Landscape for Protein Folding and Possible Connections to Function", *Polymer, 45*, 547-555 (2004).

4. M. S. Cheung, J. M. Finke, B. Callahan, J. N. Onuchic, "Exploring the interplay of topology and secondary structural formation in the protein folding problem", *J. Phys. Chem. B,* 107, 11193-11200 (2003).

3. C. Guo, M. S. Cheung, H. Levine, D. A. Kessler, "Mechanisms underlying sequence-independent beta-sheet formation*", J. Chem. Phys., 116*, 4353-4365 (2002).

2. M. S. Cheung, A. E. García, J. N. Onuchic, "Protein folding mediated by solvation: water expelling and formation of the hydrophobic core occurs after the structure collapse", *Proc. Natl. Acad. Sci. U. S. A., 99*, 685-690 (2002).

1. M. S. Cheung, I. Daizadeh, A. A. Stuchebrukhov, P. F. Heelis, "Pathways of Electron Transfer in E. coli DNA Photolyase", *Biophys. J.*, *76,* 1241-1249 (1999).

Review or Editorial Articles

6. M. S. Cheung, Dima, R.I., Hyeon, C. "Tribute to Dave Thirumalai", *J. Phys. Chem. B. 125*, 13831-13833 (2021).
5. M. S. Cheung, Arcus, V. "Editorial overview: Protein folding and binding: from protein folding in vitro to hierarchical assembly in vivo", *Curr. Op. Struc. Biol. 66,* VI-VII (2021).
4. M. S. Cheung, A. G. Gasic, "Towards developing principles of protein folding and dynamics in the cell", *Phys. Biol.*, *15*, 063001 (2018).

3. A. Christiansen, Q. Wang, M. S. Cheung, P. Wittung-Stafshede, "Macromolecular crowding effects on protein folding in vitro and in silico", *Biophysical Reviews, 5*, 137-145 (2013).

2. M. S. Cheung, "Where soft matter meets living matter -- Protein structure, stability, and folding in the cell", *Current Opinion in Structural Biology*, *23*, 212-217 (2013).

1. A. Samiotakis, P. Wittung-Stafshede, M. S. Cheung, "Folding, stability and shape of proteins in crowded environments: Experimental and computational approaches", *Int. J. Mol. Sci., 10*, 572-588 (2009).

Manuscripts in Preparation

1. P. Zhang, J. Nde, Y. Eliaz, N. Jennings, P. Cieplak, M. S. Cheung, "Chemistry-informed machine learning accurately predicts atomic charges of Ca^{2+} in proteins".

2. A. G. Gasic, C. Daugherty, M. S. Cheung, "Protein structural fluctuations at criticality in the temperature-pressure-crowding folding phase diagram".

3. J. Liman, C. Bueno, A. Chandrasekaran, Y. Eliaz, M. Ghane, C. Li, M. N. Waxham, G. A. Papoian, P. G. Wolynes, M. S. Cheung, "Multivalent interactions between CaMKII and actin regulate the nanoarchitecture of actomyosin networks".

Intellectual Property

1. George, A. D. & Cheung, M. S., "Graph identification of proteins in tomographs (GRIP-TOMO)," Provisional Application No. 63/353,974, (2022).

Conference Proceedings (peer-reviewed)

1. H. Nguyen, E. Rohit, J. Subhlok, E. Gabriel, Q. Wang, M. S. Cheung, D. Anderson, "An execution environment for robust parallel computing on volunteering PC grids", The 41th International Conference on Parallel Processing (2012).

2. E. Rohit, H. Nguyen, N. Kanna, J. Subhlok, E. Gabriel, Q. Wang, M. S. Cheung, D. Anderson, "A Robust Communication Framework for Parallel Execution on Volunteer PC Grids", 11th IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid 2011) program (2011).

3. M. Ghane, S. Chandrasekaran, R. Searles, M. S. Cheung, O. Hernandez, "Path forward for softwarization to tackle evolving hardware", Proc. SPIE, 10652, Disruptive Technologies in Information Sciences (2018).

4. M. Ghane, S. Chandrasekaran, M. S. Cheung, "Gecko: Hierarchical heterogeneous portable shared memory abstraction", Proceedings of the 10th International Workshop on Programming Models and Applications for Multicores and Manycores (PMAM, 2019).

5. M. Ghane, S. Chandrasekaran, M. S. Cheung, "Towards a Portable Hierarchical View of Distributed Shared Memory Systems: Challenges and Solutions", The 11th International Workshop on Programming Models and Applications for Multicores and Manycores (PMAM, 2020).

Membership in Professional Societies
Biophysical Society, American Physical Society, Physics Teacher Education Coalition, American Chemical Society, and Protein Society.

Services in Professional Societies
American Physical Society:

- Organizer: Focus session on "Hydrophobic Interactions in Multiple Scales for Biology" at the Annual March Meeting of the American Physical Society (2008)
- Organizer: Focus session on "Simulations and Theories for Biomolecules under Cell-like Conditions" at the Annual March Meeting of the American Physical Society (2009)
- Member at large: Division of Biological Physics, American Physical Society (2010-2013)
- Past Chair/Chair line: Division of Biological Physics, American Physical Society (2020-2024)

Biophysical Society:

- Organizer: Member-organized session on "Biopolymer Dynamics in Cell-like Environment" at the Annual Meeting of the Biophysical Society (2010)
- Founding Chair and Chair: Biopolymers In Vivo Subgroup, Biophysical Society (2011-2012)
- Member: Education Committee, Biophysical Society (2012-2015)
- Program Chair: Biopolymers *in vivo* Subgroup of the Biophysical Society Meeting (2016-2017)
- Member at large: Biopolymers *in vivo* Subgroup of the Biophysical Society Meeting (2018-2021)
- Member: Biophysical Society Council (2023-2026)

The Protein Society

- Member: Executive Council, the Protein Society (2021-2024)

Greater Science Community:

- Co-Director and faculty advisor: Science Teacher Equity Program (UH) for science teachers in elementary schools and for physics teachers in high schools (2012-2017)
- Faculty member of the steering committee: Houston Area Molecular Biophysics Training Program (2013-2020)
- Outreach Director: Center for Theoretical Biological Physics at Rice University (2013-2021)
- Chair: Protein Folding Dynamics -- from protein folding *in vitro* to hierarchical assembly *in vivo*, Gordon Research Conference (2020)
- Co-Organizer, National Science Foundation Virtual Workshop: Growing Equity, Inclusion, and Diversity for the Physics of Living Systems Student Research Network (2020).
- Faculty mentor of the Physics of Living Systems Student Research Network (2014-present).
- Faculty mentor of the Physics of Living Systems Physics Teacher Network (2020-2021).

Journal Editorial Boards and Reviewer:

- Editorial Board, *Biophysical Journal,* (2018-2023).
- Guest Editor, *The Journal of Physical Chemistr*y's Special Issue entitled: Dave Thirumalai Festschrift (2021).
- Guest Editor, *Current Opinions in Structural Biology* - Folding and Binding, Vol. *66* (2021).

- Guest Editor, *The Journal of Physical Chemistr*y's Special Issue entitled: Jose' Onuchic Festschrift (2022).
- Guest Editor, *Protein Science's* Early Career Special issue (2023).
- Associate Editor, *Reviews of Modern Physics* (2014-2022).
- Referee for Journals: *Biophysical Journal, Proteins: Structure, Function, and Bioinformatics, Protein Science, Proceedings of the National Academy of Sciences, Physical Biology, Journal of Physical Chemistry B, International Journal of Molecular Sciences, Physical Review E, Biochemistry and Cell Biology, PLoS Computational Biology, and Nano Letters.*
- Reviewer for funding agencies: National Science Foundation, Department of Energy, and American Chemical Society Petroleum Research Fund

Professional Development and Training

- UH ADVANCE Administrative Fellow (2017-2018)
- Faculty Workshop: Managing Mentoring Conversations (2019)
- UH Cougar Chairs Leadership Academy (2019-2020)

University Committee Duties at the University of Washington at Seattle (UW)
University:

- Chair of the Faculty Mentor Committee for the UW Louis Stokes Alliance for Minority Participation (UW-LSAMP, 2021-present)

Department:

- Local organization committee of the APS Conferences for Undergraduate Women in Physics (CUWiP23) (2022-2023)

University Committee, Administrative Duties, and Teaching at the University of Houston
Department:

- Website Committee (2007-2012)
- Graduate Studies Committee (2007-2013)
- Faculty Search Committee (Biophysics 2010, Nano 2014)
- Chair of the Faculty Search Committee in Biological Physics (2015)
- Personnel Committee (2012-2017)
- Chair of the Seminar Committee (2012-2017)
- Award Committee (2017-2019)
- Outreach Committee (2013-2020)
- Seminar Committee (2019-2020)
- Executive Committee (2017-2020)

College:

- College Dean Search Committee (2013-2014)
- College Strategic Planning Committee (2015)
- The Junior Faculty Award Committee (2017)

University:

- Internal Advisor Board for the Center for Advanced Computing and Data Systems (2016-2017)
- The Quality Enhancement Plan (2017-2019)
- Committee on Distinguished and Named Professorships and Chairs (2019-2020)
- Committee on Racial Equity and Social Justice (2020)

Teaching

- University of Houston Introductory General Physics I (PHYS) 1301 *Lecture-based learning*
- University of Houston Introductory General Physics I (PHYS) 1301 *Inquiry-based learning*
- University of Houston Introductory General Physics II (PHYS) 1302
- University of Houston University Physics II (PHYS) 1322
- University of Houston Thermal Physics (PHYS) 3327
- University of Houston Statistical Physics (PHYS) 6327
- University of Houston Biological Physics (PHYS) 7339

Mentored DOE Trainees, Students, and Post-docs

DOE/Science Undergraduate Laboratory Internships (SULI) trainees:
Briana Sobecks (Chem Eng, University of Illinois at Urbana-Champaign, Summer 2021)
Jose' Villalobos (Physics, University of Texas at San Antonio, Spring 2022)
Liam Mackey (Physics, Rensselaer Polytechnic Institute, Fall 2022)
Arsam Firoozfar (Computer Science, Lake Washington Institute of Technology, Summer 2023)

DOE/Community College Internships (CCI) trainees:
Ian Gildea (Engineering, Tidewater Community College, Spring 2022)
Arsam Firoozfar (Computer Science, Lake Washington Institute of Technology, Summer 2022)
Kate Baldwin (Artificial Intelligence, Bellevue College, Fall 2023)

Postdoctoral Associates:
Dirar Homouz (June 2007 – May 2009)
Current: *Associate Professor, Khalifa University (KUSTAR) in Abu Dhabi, UAE*
Balamurugan Desinghu (February 2012-August 2014)
Current: *High-performance Computing Consultant, Computational Institute, University of Chicago*
Victor M.-Y. Tsai (September 2014-August 2015)
Current: *Assistant Professor, Tamkang University, Taiwan*
Swarnendu Tripathi (August 2012-March 2016)
Postdoctoral Fellow of the Computational Cancer Biology Training Program
Current: *Bioinformatics Analyst, Medical College of Wisconsin*
Oleg Starovoytov (January 2015-December 2016)
Jaebeom Han (September 2018-May 2020)

Graduate students:
Antonios Samiotakis (UH Physics, Ph.D. 2011)
Robert S. Hyer Research Award 2010
Current: *Principal Scientist at Zymeworks*
Qian Wang (UH Physics, Ph.D. 2012)
Current: *CTBP Postdoctoral Fellow, Rice University*

Pengzhi Zhang (UH Physics, Ph.D. 2016)
Research Scientist, UH
Fabio Zegarra (UH Physics, Ph.D. 2018)
Recipient of a travel award from the Biophysical Society, 2016
Current: *Associate Professor at the National Technological University of South Lima, Peru*
Millad Ghane (UH Computer Science, Ph.D. 2019), co advised with Dr. Larry Shi
Current: *Senior Engineer at Samsung*
Jake Ezerski (UH Physics, Ph.D. 2020)
Houston Area Molecular Biophysics Training Program fellowship, 2015-2018
Winner of the best predoctoral poster presentation award at the Annual Keck Conference, 2015.
Current: *Mathematics Specialist at Start-up Clothing Tech LLC*
Yossi Eliaz (UH Physics, Ph.D. 2020)
CACDS fellow, 2017-2018
Andrei Gasic (UH Physics, Ph.D. 2020)
Recipient of the GRC Carl Storm Underrepresented Minority Fellowship 2016.
Houston Area Molecular Biophysics Training Program fellowship, 2016-2019
Robert S. Hyer Research Award 2019
Jacob Tinnin (UH Physics, Ph.D. 2022)
James Liman (Rice Bioengineering, Ph.D. 2023)
Jules Nde (UW Physics, 2019-present)
Chengxuan Li (UW Physics, 2019-present)
Jiayi Wang (UW Physics, 2022-present)

Guoxiong Su (UH Physics, M.S. 2012)
Houston Area Molecular Biophysics Training Program (non-funded) fellowship, 2011-2012
Jianfa Chen (UH Physics, M.S. 2014)
Mohammadmehdi Ezzatabadipour (UH Physics, M.S. 2016)
Hoa Lan Trinh (UH Physics, 2016-2018)
Tim Burt (UH Physics, 2018-2019)
Atrayee Sarkar (UH Physics, 2020-2021)

Undergraduate students:
Marc Gonzalez (Physics, Summer 2007)
Byron Hoffman (Physics, Summer 2008)
His work was acknowledged by coathorship in a research article
Nathaniel Morgan (Physics, Fall 2008-Spring 2009)
Syed Razavi (Chem and Biomolecular Engineering, Summer 2009)
Rizwan Tai (Political Sci., Summer 2009)
Faheem Shahid (Mechanical Engineering, Summer 2009)
Tyler Quarton (Biochemistry, Fall 2009)
Brian Bush (Physics, Fall 2009)
Megan Scoppa (Biochemistry, Spring 2009-Spring 2011)
Recipient of NSF REU award, Summer 2010
Ian Mitchell (Physics, Summer 2010)
Recipient of Summer Undergraduate Research Fellowship, Summer 2010
Ashlynne Monroe (Health, Spring 2010-Spring 2011)
Sana Mateen (Chemical Engineering, PURS Fall 2011)
Recipient of Provost Undergraduate Research Fellowship, Fall 2011

Gabriela Bernardes (Mechanical Engineering, Summer 2011-Spring 2012)
Her work was acknowledged by coathorship in a research article
Francis de Dios (Physics, Summer 2012-Spring 2013)
Recipient of Provost Undergraduate Research Fellowship, Fall 2012
Lionel Flores (Physics, Summer 2012-present)
Recipient of NSF REU award, Summer 2012
Recipient of CTBP REU award, Summer 2013
Nicole Davidson (Physics, Summer 2013)
Recipient of CTBP REU award, Summer 2013
Lenaya Flowers (Physics, Summer 2014-Fall 2015)
Recipient of CTBP REU award, Summer 2014
Rodney Helm (Physics, Summer 2014-Summer 2016)
Recipient of CTBP REU award, Summer 2014
Sarai Vargas (Biology, Fall 2015-Spring 2016)
Recipient of CPRIT undergraduate research fellowship in computational cancer biology, Summer 2016
Marissa Soto (Physics, Summer 2016-December 2017)
Recipient of Physics Undergraduate Fellowship, Fall 2016
Caleb Daugherty (Physics, Summer 2016-December 2017)
Recipient of CTBP REU award, Summer 2016
His work was acknowledged by coathorship in a research article
Luis H. Victor (Physics, Spring 2017-Summer 2017)
Recipient of CTBP REU award, Summer 2017
Lucas Babel (Physics, Fall 2017-Summer 2019)
Recipient of CTBP REU award, Summer 2018
His work was acknowledged by coathorship in a research article
Brett Velasquez (Physics, Summer 2017-Spring 2020)
Recipient of CTBP REU award, Summer 2017
Nate Jennings (Physics, CMU, Summer 2019, Summer 2020)
Fardowsa Douled (Informatics, UW, Summer 2023)
Eve Johnson (Physics and Astronomy, UW, Summer 2023-present)
Malio Nelson (Comprehensive Physics, UW, Winter 2024-present)

Selected Invited Talks (in reverse chronological order)

- Graph Identification of Proteins in Tomograms, Contributed talk, The American Physical Society March Meeting, March 2023.
- Emergent Protein Assemblies in vivo, Invited talk, Biopolymers in vivo Subgroup, Biophysical Society Annual Meeting, February 2023.
- Graph Identification of Proteins in Tomograms, Data Modeling and Computation: Capturing Biomolecular Processes, CECAM, Lausanne, Switzerland, November 2022
- From Protein Folding in a Crowd to Higher-order Assemblies in a Cell, Keynote, Gordon Research Conference, Protein Folding Dynamics, Ventura, CA, October 2022.
- Proteins in a Crowd under Heat and Pressure, Biophysics Seminar, Center for Biological Physics, University of California at Los Angeles, virtual, May 2022.
- Proteins in a Crowd under Heat and Pressure, Biological Physics/Physical Biology seminar, virtual, April 2022.
- Understanding Protein Complex Assembly through Grand Canonical Maximum Entropy Modeling, Contributed talk, The American Physical Society March Meeting, March 2022.

- Proteins in a Crowd under Heat and Pressure, Physics Colloquium University of Idaho, virtual, October 2021.
- Proteins in a Crowd under Heat and Pressure, Biostatistics Seminar, University of Kansas Medical Center, virtual, October 2021.
- The Dual Role of Calcium/Calmodulin-dependent kinase II in transducing calcium signals and reorganizing actomyosin networks, Invited talk, The American Physical Society March Meeting, March 2021.
- Physics of Memory and Learning – from the Perspective of Biomolecules, The Penn Muscle Institute Seminar, University of Pennsylvania, virtual, December 2020.
- From Protein Folding *in vitro* to Hierarchical Assembly *in vivo*, Laufer Center for Physical and Quantitative Biology Seminar, Stony Brook University, virtual, December 2020.
- From Protein Folding *in vitro* to Hierarchical Assembly *in vivo*, Physical Chemistry Seminar, University of Washington, virtual, October 2020.
- Physics of Memory and Learning – from the Perspective of Biomolecules, Seminar, Molecular Engineering, University of Washington, virtual, October 2020.
- Proteins in a Crowd under Heat and Pressure, Physics Colloquium, University of Washington, virtual, October 2020.
- From Protein Folding *in vitro* to Hierarchical Assembly *in vivo*, Pacific Northwest National Laboratory, virtual, July 2020.
- Assemblies of Calcium/Calmodulin Dependence Kinase II with Actin and their Dynamic Regulation by Calmodulin in Dendritic Spines, Virtual 2020 Annual March Meeting, American Physical Society, 2020.
- Proteins in a Crowd under Heat and Pressure, Symposia, Biophysical Society Annual Meeting, San Diego, CA, February 2020.
- Proteins in a Crowd under Heat and Pressure, Physics Colloquium, University of Florida, Gainesville, FL, February 2020.
- Proteins in a Crowd under Heat and Pressure, Inaugural Speaker, Rice Women in Physics Distinguished Lecture Series, Rice University, Houston, TX, February 2020.
- Critical Phenomena in the Temperature-Pressure-Crowding Phase Diagram of a Protein, Biophysics Seminar, Ohio State University, November 2019.
- Physics of Memory and Learning – from the Perspective of Biomolecules, Biophysics Seminar, University of Maryland, October 2019.
- Critical Phenomena in the Temperature-Pressure-Crowding Phase Diagram of a Protein, 2019 Taipei International Workshop for Soft Matter and Biophysics, Taipei, Taiwan, September 2019.
- Physics of Memory and Learning – from the Perspective of Biomolecules, The 19th KIAS Conference on Protein Structure and Function, Seoul, Korea, September 2019.
- Critical Phenomena in the Temperature-Pressure-Crowding Phase Diagram of a Protein, The Fourth International Conference on Computational Science and Engineering, Ho Chi Minh City, Vietnam, July 2019.
- Critical Phenomena in the Temperature-Pressure-Crowding Phase Diagram of a Protein, Macromolecular Crowding Telluride Science Research Center, Telluride, CO, July 2019.
- Critical Phenomena in the Temperature-Pressure-Crowding Phase Diagram of a Protein, 33rd Protein Society Annual Meeting, Seattle, WA, July 2019.

- Physics of Memory and Learning – from the Perspective of Interacting Molecules, Physics Colloquium, University of Houston at Clear Lake, Houston, TX, March 2019.
- Physics of Memory and Learning – from the Perspective of Interacting Molecules, Outreach Seminar, Houston Community College, Houston, TX, February 2019.
- Physics of memory and learning – from the perspective of interacting molecules, Physics Colloquium, University of Houston, Houston, TX, November 2018.
- Molecular underpinnings of postsynaptic calmodulin dependent Ca^{2+} signaling, plenary speaker, Texas Section of the APS, Houston, TX, October 2018.