John W. Craft, Jr.

University of Houston
Dept. Biology and Biochemistry
Box 90097/ HSC 358
Houston, TX 77204-5001

https://www.uh.edu/~jwcraft/
Cell: (281) 538-1219
Email: jwcraft@uh.edu
Email: jjwwcraft@gmail.com

EDUCATION

2009 Ph.D. Biochemistry, Chemical Biology,
Department of Biology and Biochemistry, University of Houston
Dissertation: NMR LINE BROADENING AS A SIGNATURE OF CHEMICAL EXCHANGE AND ENTROPIC PRIMING Advisor: Dr. Glen B. Legge

1990 B.S. Aerospace Engineering, Wichita State University Cum Laude with Honors
Honors: Wallace, Rodgers, McGregor, Fugate, Hutton, and Johnson Scholarships.
Honors: Emory Lindquist Honors Recipient.

PROFESSIONAL EXPERIENCE

2023–present University of Houston Department of Biology and Biochemistry
Research Associate Professor

2017-present *Research Consultant*: KRATON POLYMERS; computational material/chemistry

2015-present Dual Researcher: Texas Heart Institute, Houston Texas

2015–2023 University of Houston Department of Biology and Biochemistry
Research Assistant Professor

2009-2014 Postdoctoral Research Scientist, UH

2003-2009 Research Assistant, UH

1992-2002 **NASA** Johnson Space Center
Shuttle Ascent Guidance, Navigation, and Control **Technical Chairman**

- Honors: **Silver Snoopy** for outstanding achievements related to flight safety. Presented personally by astronauts to **less then 1%** of eligible recipients (1996)
- Space Flight Awareness Award (1998)
- Engineering Support Commendation MS4-98-014 (1998)

Technical and programmatic manager of prime contract areas related to ascent GN&C. Lead manager for 7 to 15 engineers and a multi million-dollar budget responsible for independent verification of certification and flight products.

1988-2002 NASA Johnson Space Center, Aerospace Engineer, **Clear Case Software Lead; *Supported 113 Launches***,

Principle Function Owner for Space Shuttle Systems:

- Ascent Digital Auto Pilot (DAP), Ascent First Stage Guidance,
- Ascent Second Stage Guidance, Return to Launch Site (RTLS) Guidance
- Monte Carlo for large-scale spacecraft. Modified the hardware in the loop, man in the loop, Shuttle Engineering Simulation (SES) for the X-38 re-entry manned spacecraft.
- Flexible Airframe Response (FAR) flight control Monte Carlo of STS-93 ascent/payload for the flight readiness evaluating flexible structure and slosh fluid flight control margins.
- Non-linear describing function analysis for the Coulomb Dampers for the Chandra X-ray Telescope payload.
- Manager and lead developer for the SES for X-38 and US Space Shuttle.
- ***MANY: Software Requirement; Updates, DR's, Test Analysis, Certification Reports.***

PUBLICATIONS

Selected Publications in Refereed Journals (17) (3 2021; 1 2022; 1 in 2023)

1. Reyes-Alcaraz A, Qasim H, Merlinsky E, Fox G, Islam T, Medina B, Schwartz RJ, **Craft JW Jr**, McConnell BK. A Small Molecule That In Vitro Neutralizes Infection of SARS-CoV-2 and Its Most Infectious Variants, Delta, and Omicron. **Biomedicines**. (**2023)** Mar 15;11(3):916. doi: 10.3390/biomedicines11030916. PMID: 36979895; PMCID: PMC10046252.
2. Hickman A, Koetsier J, Kurtanich T, Nielsen MC, Winn G, Wang Y, Bentebibel SE, Shi L, Punt S, Williams L, Haymaker C, Chesson CB, Fa'ak F, Dominguez AL, Jones R, Kuiatse I, Caivano AR, Khounlo S, Warier ND, Marathi U, Market RV, Biediger RJ, **Craft JW Jr**, Hwu P, Davies MA, Woodside DG, Vanderslice P, Diab A, Overwijk WW, Hailemichael Y.; LFA-1 activation enriches tumor-specific T cells in a cold tumor model and synergizes with CTLA-4 blockade. **J Clinical Invest. (2022)** Jul 1;132(13):e154152. doi: 10.1172/JCI154152
3. Lydia R. St. Hill, Hung-Vu Tran, Pawilai Chinwangso, Han Ju Lee, Maria D. Marquez, **J.W. Craft, Jr.** and T. Randall Lee; Antifouling Studies of Unsymmetrical Oligo(ethylene glycol) Spiroalkanedithiol Self-Assembled Monolayers; **MACRO (2021)**
4. Lydia R. St. Hill, **J.W. Craft, Jr**, P Chinwangso, H Tran, M.D. Marquez and T.R. Lee; Antifouling Coatings Generated from Unsymmetrical Partially 2 Fluorinated Spiroalkanedithiols; **ACS Applied Bio Materials** Feb 1 **(2021)** doi.org/10.1021/acsabm.0c01409
5. D Bakthavatsalam, **J.W. Craft Jr.**, A Kazansky, N Nguyen, G Bae, A.R. Caivano1, C.W. Gundlach IV, A Aslam, S Ali, S Gupta, S.Y. Lin, H.D. Parthiban, P Vanderslice, C.C. Stephan and D.G. Woodside; Identification of Inhibitors of Integrin Cytoplasmic Domain Interactions With Syk; **Front. Immunol.,** 08 January **(2021)** 10.3389/fimmu.2020.575085
6. Reza Abbasgholizadeh, Hua Zhang, **J.W. Craft Jr,** Robert M Bryan Jr, Steven J Bark, James M Briggs, Robert O Fox, Anton Agarkov, Warren E Zimmer, Scott R Gilbertson, Robert J Schwartz. Discovery of vascular Rho kinase (ROCK) inhibitory peptides. **Exp Bio Med (2019)**
7. K Kurakula, DS Koenis, MA Herzik Jr., Y Liu, **J.W. Craft Jr.,** PB van Loenen, M Vos, MK Tran, HH Versteeg, MTH Goumans, W Ruf, CJM de Vries, M Şen, "Structural and cellular mechanisms of peptidyl-prolyl isomerase Pin1-mediated enhancement of Tissue Factor gene expression, protein half-life, and pro-coagulant activity." **Haematologica. (2018)**
8. D.G. Woodside, E.A. Tanifum, K Ghaghada, R.J. Biediger, A.R. Caivano, Z.A. Starosolski, S. Khounlo, S. Bhayana, S. Abbasi, **J.W. Craft Jr**., D.S. Maxwell, C. Patel, I.V. Stupin, D. Bakthavatsalam, R.V. Market, J.T. Willerson, R.A.F. Dixon, P. Vanderslice, A.V. Annapragada. Magnetic Resonance Imaging Atherosclerotic Plaque at Clinically Relevant Field Strengths (1T) by Targeting the Integrin α4β1. **Science Reports: (2018).**
9. P Cherubin, MC Garcia, D Curtis, CB Britt, **J.W. Craft Jr**., H Burress, C Berndt, S Reddy, J Guyette, T Zheng, Q Huo, B Quiñones, JM Briggs, K Teter. Inhibition of Cholera Toxin and Other AB Toxins by Polyphenolic Compounds. **PLoS One.** Nov 9;11(11), **(2016)**
10. **J.W. Craft Jr.,** T. Shen, L. M. Brier, and J. M. Briggs. Biophysical Characteristics of Cholera Toxin and Escherichia coli Heatlabile Enterotoxin Structure and Chemistry Lead to Differential Toxicity. **J Phys Chem B, (2015).**
11. **J.W. Craft Jr.**, H. Zhang, M. N. Charendoff, J. T. Mindrebo, R. J. Schwartz, J. M. Briggs. Associations between the Rho kinase-1 catalytic and PH domain regulatory unit. **J Mol Graphic Model,** 46: 74-82 **(2013)**.
12. A. Rababa'h, J.W. Craft Jr., C.S. Wijaya, F. Atrooz, Q. Fan, S. Singh, A.N. Guillory, P. Katsonis, O. Lichtarge, B.K. McConnell. Protein Kinase A and Phosphodiesterase-4D3 Binding to Coding Polymorphisms of Cardiac Muscle Anchoring Protein (mAKAP). **J Mol Biol,** S0022- 2836(13)00393-8 **(2013).**
13. N.C. Anastasio, S.R. Gilbertson, M.J. Bubar, A. Agarkov, S.J. Stutz, Y. Jeng, N.M. Bremer, T.D. Smith, R.G. Fox, S.E. Swinford, P.K. Seitz, M.N. Charendoff, **J.W. Craft Jr**, F.M. Laezza, C.S. Watson, J.M. Briggs, K.A. Cunningham. Peptide inhibitors disrupt the serotonin 5-HT2C receptor interaction with phosphatase and tensin homolog to allosterically modulate cellular signaling and behavior. **J. Neurosci,** 1615-30 **(2013).**
14. R. Carreno, W.S. Brown, D. Li, J.A. Hernandez, Y. Wang, T.K. Kim, **J.W. Craft Jr**., K.V. Komanduri, L. Radvanyi, P. Hwu, J.J. Molldrem, G. B. Legge, B.W. McIntyre, and Q. Ma. 2E8 Binds to the High-Affinity I-domain in a Metal Ion Manner: A Second Generation Monoclonal

Antibody Selectively Targeting Activated LFA-1. **J. Biological Chemistry**, M110.111591 **(2010).**

15. M. Sen, M. Herzik, **J.W. Craft Jr**., A.L. Creath, S. Agrawal, W. Ruf, and G. B. Legge. Spectroscopic characterization of successive phosphorylation of the tissue factor cytoplasmic region. **Open Spec J**, 3:58-64 (**2009**)
16. R.S. Ampapathi, A.L. Creath, D.I. Lou, **J.W. Craft Jr**., S.R. Blanke, and G.B. Legge. Order-disorder-order transitions mediate the activation of cholera toxin. J Mol Biol, 377:748-760 (**2008**).
17. **J.W. Craft Jr**. and G.B. Legge. An AMBER/DYANA/MOLMOL phosphorylated amino acid library set and incorporation into NMR structure calculations. J Biomol NMR, 33:1524 (**2005**).
18. **J.W. Craft Jr**. Craft J, et. al. Flight Readiness Review (FRR) for STS-93 Flight Control Redesign Phased Performance Enhancement Implementation for payload Chandra X-Ray Telescope. (**1999**). (and many more)
19. **Craft JW Jr.**, et. al.. STS 83-0008-26 Space Shuttle Orbiter Operational Level C Functional Subsystem Software Requirements; Guidance, Navigation, and Control; Part C, Flight Control - - Ascent Flight Phase Volume 1. Houston, TX: NASA Space Shuttle Program; **(1998)**. OI-26 and OI-26B FSSR: Flight Software for Performance Enhancements. (and many more)

PATENT APPLICATIONS, DISCLOSURES AND SCIENTIFIC SOFTWARE

1. *"Small molecules that treat or prevent viral infections"*; # PCT/US23/18111210 #: AF23853-P181V1; 21-Feb-2022); Date: 17-Feb-2023; Inventors: Bradley K. McConnell, Arfaxad Reyes-Alcaraz, **John W. Craft, Jr.,** and Robert J. Schwartz
2. Provisional: Small Molecules That Treat or Prevent Viral Infections **63/312,351**; Feb 21, **2022**
3. Patent: Rho Associated Kinase (ROCK) Inhibitors and Their Use in Treating Disease, **62/060,336**, Oct 6, **2014**.
4. Inhibition of Rho Associated Kinase, Office of Research, University of Houston **UH2014-55**.
5. Phosphorylated Amino Acid Library: http://www.bchs.uh.edu/glegge/phospho lib/index.html
6. Patent: M. Hammerschmidt, J. W. Craft, Jr., Ascent/Entry Shuttle Engineering Simulation (A/E SES), software patent and release NASA Case No: **MSC-24692**

INVITED TALKS and BRIEFINGS/REPORTS

1. PolyFTS and Predici in Practical Industrial Applications and Future Prospects in an AI Agentic World, **Complex Fluids Design Consortium University of California Santa Barbara**, John W. Craft, Jr., (**1/30/2026**)
2. From Rocks to Rockets; Therapeutics, and New Materials, John Craft, Jr., Instituto Tecnologico Superior de Zacapoaxtla, **Zacapoactla Mexico**; Oct 20, (**2021**)
3. Leveraging Simulations in Therapeutics and Diagnostics; John Craft, Jr., Elizabeth Merlinsky, Ashley Cruz; UH Hewlett Packard Enterprise Data Science Institute; Nov 12, (**2020**)
4. Insights into Biophysical Characteristics of Cholera Toxin and Other AB5 Toxins and Applications to Drug Design, J. W. Craft, Jr., University of Central Florida, Biophysics Seminar (**2015**)

Dr. Craft has been foundational in the deployment of computational chemistry behind the corporate veil at Kraton since 2017. Especially solving engineering problems through the analysis of data generated from tools like; PolyFTS, LAMMPS, GROMACS, Gaussian16, and others. Dr. Craft is very motivated to see the development of resilient AI agentic systems to protect intellectual property and allow us to improve productivity in the AI generation. He developed these computational workflows that span molecular dynamics (MD) simulations {LAMMPS/GROMACS}, quantum mechanics calculations {Gaussian16}, and self-consistent field theory energy (Hamiltonian) minimizations {PolyFTS}. Internally published reports for which some data is IP protected:

1. Quantitative Structure-Activity Relationships of Kraton Resins (2019)
2. TriBlock-Copolymer Melt Phase Map (2019)
3. Evaluation of G1701 and (Branched)-arm Block-Copolymers that Form Micelles in Oil using POLY-FTS (2020)
4. MD6951 Tolerances (2021)
5. PPO-SEBS Blends {Computational Component}(2021)
6. NANO Morphologies (2024)
7. Examining Possible Mechanism for Decoupling Using Quantum Mechanics: Gaussian16 Studies (2024)

UNIVERSITY OF HOUSTON SEMINARS

1. The Ghost in the Machine; Translating Computational Lift into Experimental Validation and Intellectual Property, University of Houston Biology and Biochemistry Retreat; John W. Craft, Jr., (**3/6/2026**)
2. Pharmacophore Models and Drug Discovery for the Inhibition of Rho Kinase-1 (ROCK1) in Heart Disease and Rheumatoid Arthritis, J. W. Craft, Jr., (**2010**)
3. LFA1 High Affinity NMR Studies, J. W. Craft, Jr., Biochemistry Graduate Lecture (**2007**)

GRANTS FUNDED

1) **R61 HL168737** (PI:Woodside/**Co-PI:Craft**) 06/01/2023 - 06/01/2026
NIH/NHLBI Total Award Amount (including Indirect Costs): $1,725,687.00
- "Targeting Integrin Signaling in Atherosclerosis"
- Goal: Identifying small molecule antagonists of integrin signaling in leukocytes that can be used to target residual inflammatory risk in patients with cardiovascular disease.

2) **R44 DK127869** (PI:Woodside) 07/2023 - 06/2025 **Role: researcher**
NIH/NIDDK (total) $2,293,047
- "Selective targeting of high affinity alpha4 integrins as a safe treatment strategy for IBD"

3) **R01 AI137056-01** (PI:Teter/**Co-PI:Craft**) 04/01/2018 - 08/31/2023
NIH/NIAID Score 4% (total) $1,828,727 / (Craft) $114,752
- "The "Disaggregase" Mechanism of Holotoxin Disassembly by Protein Disulfide Isomerase"
- Goal: Elucidate protein disulfide isomerase (PDI)-mediated Cholera holotoxin disassembly.

4) **R41 DK127869** (PI:Woodside) 09/2020 - 09/2022 **Role: researcher**
NIH/NIDDK (added to #2)
- "Selective targeting of high affinity alpha4 integrins as a safe treatment strategy for IBD"

5) **Kraton: 63486** (**PI: Craft**) 06/25/2018 - 9/31/2026
Unrestricted Gift to the PI $415,000
- Goal: To advance the computational predictions of material properties and morphologies of advanced block copolymers. Understand the partition tendencies of complex mixtures of polymers in oils or solvents.

6) **Texas Heart Institute**: (**PI: Craft**) 01/01/2015 - 12/31/2026 $226,000
- Goal: To advance the computational simulations of lead compounds that could lead to therapeutics in inflammation, inflammatory bowel disease, and Crohn's.

7) **AHA 18AIREA33960175** 07/01/2018 – 12/30/2021
American Heart Association (PI: McConnell/**Col Craft**) $154,000
- "Gravin Signalosome Mediates Cardiac Signaling and Transcriptome Variation in Heart Failure"

- Goal: Determine the protein structural mechanisms responsible for gravin binding to the β2-AR in order to establish a functional basis for rational drug design.

8) **GEAR ON COVID-19** AND THE **GEAR ON PANDEMIC** (account #**C0505773**)
(PI: McConnell / **CoI Craft**) 9/1/2020 - 12/31/2021 $178,969
- "Screening and Compound Synthesis towards Therapeutic Modulation of Inflammation due to SARS-CoV-2"
- Goal: Find new therapeutic leads against SARS-Cov-2

9) **Microsoft CRM:0740135** (**PI: Craft**) 10/7/2017 -6/7/2022
Microsoft Azure Research Award $25,000
- "South BD Hub Targeting Simultaneous Multi-Effectors in Integrin Signaling Pathways"
- Goal: Establish a big data work flow for analysis of complexes and search for mechanisms to modulate protein signaling with high performance computing.

10) **SeFAC: 63445-B5006** (**PI: Craft**) 8/7/2018 - 4/30/2020
Center for Advanced Computing and Data Science Award $50,000
- "Targeting Multi-Effectors in SYK/Integrin Signaling Pathways"
- Goal: Autodock and Molecular Dynamics Simulations to discovery lead compounds that inhibit SYK, Talin, or Integrin signaling. Develop a candidate list of drug leads for Texas Heart Institute to test and validate.

11) **UH NFRG 111208** (**PI: Craft**) 9/1/2015 - 10/31/2016
University of Houston New Faculty Research Grant $6,000
- "Regulation of Regeneration and Remodeling of Tissues in the Heart"
- Goal: Perform a rational drug discovery computational analysis of small molecules that target hippo pathway proteins; Salv, MOB, Merlin. Perform molecular dynamics analysis of the Pin-WW domain interactions with Tissue Factor.

12) **NHARP 003652- 0213-2009** **Role: Key Personnel**
(PI: Dr. Schwartz)
- "Novel Rho Kinase Inhibitor Therapy for Cardiovascular Disease"

GRANTS PENDING

---

1) **DE-FOA-0003612 GENESIS, DOE** $750,00 **Role: PI**
"Maximizing Scale and Minimizing Time to Market for Material Descovery in an AI Agentic World"
2) **R41 A1000000-00, NIH/NCI** $399,215 **Role: Co-Investigator**
Holland, Vanderslice (Co-PIs),
- "Engineering a conformationally independent VLA-4 antagonist for hematopoietic stem cell mobilization"

3) **AMAZON Proposal ID: 19208** $80,000 + $40,000 credits **Role: PI**
- "Secure Agentic AI Framework for Molecular Modeling and Quantum Mechanics Workflows"

4) **GEAR 2026** $36,544 **Role: PI**
- "Talin as a Signaling Node in Integrin Regulation of Inflammation and Focal Junctions"

5) **Crohn's Foundation 2026** $130,000 **Role: Co-PI**
Woodside (PI) 9/1/2026 - 10/31/2028 $130,000
- " α4-integrin targeted nanoparticle as a theranostic for Inflammatory Bowel Disease"
- Goal: Modification of integrin a4ß1/a4ß7 dual specificity small molecule compounds for incorporation into lipid-based nanoparticles. Develop integrin a4ß1/a4ß7 targeted nanoparticles with imaging and drug delivery functionalities. Modified a4ß1/a4ß7 antagonists will be incorporated into lipid-based nanoparticles (LNPs).

6) **American Heart Association 2026** $200,000 **Role: Co-I**
Woodside (PI)
- "Bispecific Engagers for Atherogenic Lipoproteins"

- Goal: Development of a Bispecific LDLR-engager (BiLR-E) to clear atherogenic lipoproteins such as oxLDL and L5 from circulation. Creating a bi-specific biologic that is comprised of the extracellular domain of LOX-1, which binds both oxLDL and L5, fused to a nanobody that binds the extracellular domain of LDLR .

GRANTS SUBMITTED BUT NOT FUNDED

1) **UH Drug Discovery Institute** 07/01/2025 – 12/31/2026 **Role: PI**
$50,000

- "Targeting the A-Kinase Anchoring Protein (AKAP-12) signalosome"
- Goal: Identifying new therapeutic interventions to block AKAP-12 binding to β-adrenergic receptor to disrupt β2-AR desensitization is critical to cardiac signaling in heart failure.

2) **R01 EB026054-01** 04/01/2018 – 03/31/2023 **Role: PI**
$1,912,500

- "Trojan Horses for Protein Cargo Delivery"
- Goal: Develop novel synthetic biological systems to retro-translocate proteins cargos using modified AB5 toxin subunits or LFA-1 Coated Silicon Nanoparticles.

3) **R01- AI141781** 10/01/2018 -- 09/30/2023 **Role: PI**
NIH/NIAID: $1,910,866

- "Borrelia Burgdorferi Proteins on the Host/Pathogen Interface in Lyme Disease"
- Goal: Develop and Test Lead Inhibitors to Interdict in Lyme Disease

4) **R21 EB025940-01** 04/01/2018 – 03/31/2021 **Role: PI**
NIH/ NIBIB 12.0 Cal $125,000
NIBIB TRAILBLAZER AWARD FOR NEW AND EARLY STAGE INVESTIGATORS (R21)

- "Bioengineering Polymer Matrix Challenges Simulation Scale: A Coarse Grain Approach for High Dimensional Problems in BioMaterials"
- Goal: Parameterize and simulate at LARGE scale the biomaterial surface interaction and develop partially fluorinated spiroalkanedithiols with unsymmetrical geometries.

5) External 01/01/2018 - 12/31/2018 **Role: PI**
The William and Ella Owens Medical Research Foundation 12.0 Cal $100,000

- "Synthetic Protein Cargo Delivery in Cells Using Mimicry and Dosing Nanocapsules"
- Goal: Substitute the A subunit of Cholera with a synthetic protein.

6) **W81XWH-17-TBDRP-IA** 02/01/2018 – 07/31/2019 **Role: PI**
DOD 9.0 Cal $130,658

- "TB170129 Targeting Borrelia burgdorferi Membrane Proteins that Bind Human Cells in Infection of Lyme Disease"
- Goal: Develop new drugs to block Borrelia burgdorferi infection and reduce Lyme disease.

7) **PhRMA Foundation**: **Role: PI**
$100K + ($14K matching)

- "Targeting Simultaneous Multi-Effectors in Integrin Signaling Pathways for Translational Impact and Diagnostics "

8) **PRMRP W81XWH-17-PRMRP-DA** 02/01/2018 – 07/01/2019 **Role: PI**
DOD 12.0 Cal $125,000

- "PR172162 Targeting Simultaneous Multi-Effectors in Integrin Signaling Pathways"
- Goal: Develop novel "multivalent" regulators of integrin signaling can dramatically mitigate tissue remodeling in disease pathogenesis and Develop a novel bi-direction switch using SYK to improve health and safety.

9) **PRMRP W81XWH-17-PRMRP-DA** 02/01/2018 – 07/01/2019 **Role: PI**
DOD 12.0 Cal $125,000

- "PR172261 Synthetic Protein Cargo Delivery in Cells Using Mimicry and Nanocapsules"
- Goal: Develop unique synthetic biological systems to retro-translocate proteins cargos using modified AB5 toxin subunits or LFA-1 Coated Silicon Nanoparticles.

10) **PRMRP W81XWH-17-PRMRP-DA** 02/01/2018 – 07/01/2019 **Role: Key Per**
DOD 6.0 Cal $125,000

- "Stimulating the Hippo Pathway to Induce Tissue Regeneration"
- Goal: Identify and validate lead compounds targeting proteins in the Hippo pathway

11) **UH** 02/01/2018 - 7/31/2019 **Role: PI**
High Priority Area Research Seed Grant $70,000

- "Cloud Computing Analytics for Drug Discovery"
- Goal: Deploy Drug Discovery Pipeline on the Microsoft, Amazon, and Google clouds

MY PROCEEDINGS AND POSTERS

1. **J. W. Craft, Jr.,** Amy Caivano, Anna Kazansky, Shahrzad Abbasi, Reiko Chamberlain, Qian Xiang, Anuj Kurella, Elizabeth Merlinskey, Yi Zhao, Frederick Meece, Darren Woodside, Targeting Integrin Signaling In Atherosclerotic Cardiovascular Disease (Ascvd), 13th ANNUAL SYMPOSIUM **Cardiovascular Research Institute @ Baylor College of Medicine (2026)**
2. **J. W. Craft, Jr.,** Ron Biediger, Robert Market, Frederick Meece, Amy Caivano, Anna Kazansky, Shahrzad Abbasi, Peter Vanderslice, Darren G. Woodside, Drug Discovery: Workflow and Implementation in Targeting Spleen Tyrosine Kinase/SYK, **Drug Discovery Institute Symposia** (**2025**)
3. **J. W. Craft, Jr.,** Ron Biediger, Robert Market, Frederick Meece, Amy Caivano, Anna Kazansky, Shahrzad Abbasi, Peter Vanderslice, Darren G. Woodside, Drug Discovery: Workflow and Implementation in Targeting Spleen Tyrosine Kinase/SYK, **Muscle Biology and Cachexia Conference** (**2025**)
4. **J. W. Craft, Jr.,** and R. J. Schwartz, Phosphorylation Mimicry in Espresso; Charge Gradients and Dynamics, Simulating Soft and Active Matter with ESPResSo, ESPResSo++, and VOTCA, **Stuttgart, Germany** (**2015**)
5. **J. W. Craft, Jr.,** T. Shen, L.N. Brier, and J. M. Briggs, Biophysical Characteristics of Cholera Toxin and E. coli Heat-labile Enterotoxin Structure and Chemistry Lead to Differential Toxicity, 49th US Japan Conference on Cholera and Other Enteric Bacterial Infections, **Gainsville, FL** (**2015**)
6. Abeer Rababah, **J. W. Craft, Jr**., A. Guillory, C. Wijaya, S. Singh, Q. Fan, A. D. Diaz, X. Yin and B. K. McConnell, Cardiac Scaffold Protein Binding Kinetics: A Role for Altered Signaling during Human Heart Disease, ASPET Annual Meeting at Experimental Biology**, San Diego, CA** (**2012**)
7. **J. W. Craft, Jr**., H. Zhang, M.N. Charendoff, J. M. Briggs, and R. J. Schwartz, Docking Rho Kinase 1 Catalytic and PH Domain and Inhibition in Heart Disease, 17th Annual Sealy Structure Biology Symposium at UTMB, Galveston, TX (**2012**)
8. **J. W. Craft, Jr**., H. Zhang, M.N. Charendoff, J. M. Briggs, and R. J. Schwartz, Rho Kinase 1 Complexes and Inhibition in Heart Disease, Computational and Theoretical Biology Symposium, Houston, TX (**2011**)
9. **J. W. Craft, Jr.,** H. Zhang, M.N. Charendoff, J. M. Briggs, and R. J. Schwartz, Mechanisms of Rho Kinase 1 Inhibition in Heart Disease, 5th John S. Dunn Gulf Coast Consortium for Magnetic Resonance Conference, Houston, TX (**2011**)
10. **J. W. Craft, Jr.,** H. Zhang, T. Shen, J. M. Briggs, and R. J. Schwartz, Drug Discovery for Inhibition of Rho Kinase in Heart Disease, 20th Annual Keck Research Conference, Houston, TX (**2010**)

11. **J. W. Craft, Jr.,** H. Zhang, J. M. Briggs and R. J. Schwartz, NMR in Small Molecule and Peptidomimetic Discovery for Inhibition of Rho Kinase, 4th John S. Dunn Gulf Coast Consortium for Magnetic Resonance Conference, Houston, TX (**2010**) **2nd place winner**
12. **J. W. Craft, Jr.,** H. Zhang, T. Shen, J. M. Briggs, and R. J. Schwartz, Structural Analysis of Rho Kinase in Investigations of Mechanisms in Cardiovascular Disease, 15th Annual Sealy Structure Biology Symposium at UTMB, Galveston, TX (**2010**)
13. **J. W. Craft, Jr.,** T. Shen, G. B. Legge and J. M. Briggs, Exploring Cholera Toxin and E. coli Heat-labile Enterotoxin Subunit Interactions Using Steered Molecular Dynamics, Southwest Theoretical Chemistry Conference, Houston, TX (**2009**)
14. T. Shen, **J. W. Craft, Jr**., G. B. Legge and J. M. Briggs, Exploring Cholera Toxin and E. coli Heat-labile Enterotoxin Subunit Interactions Using Steered Molecular Dynamics, **44th US-Japan Conference on Cholera and Other Bacterial Enteric Infections, San Diego, CA** (**2009**)
15. C. J. Wittkopp, **J. W. Craft, Jr**., M. E. Altunop, A. Creath, G. B. Legge, Formation of the Escherichia coli Heat Labile Toxin: Human ADP-Ribosylating Factor 6 Complex, **44th US-Japan Conference on Cholera, Other Bacterial Enteric Infections**, **San Diego, CA** (**2009**)
16. **J. W. Craft, Jr.** and G. B. Legge, NMR Isotope Filtering Techniques Applied to a Complex with Line Broadening Characteristics, 3rd John S. Dunn Gulf Coast Consortium for Magnetic Resonance Conference, Houston, TX (**2009**) **2nd place winner**
17. **J. W. Craft, Jr.** and G. B. Legge, The Role of Entropic Priming in the Activation of the LFA-1 I-domain, 13th Annual Sealy Structure Biology Symposium at **UTMB, Galveston, TX** (2008)
18. M. Herzik, M. Sen, A. Creath, **J. W. Craft, Jr.,** W. Ruf and G. B. Legge, Solution Structure of Pin1 WW Domain Complexed with Phosphorylated Tissue Factor Cytoplasmic Domain, 13th Annual Sealy Structure Biology Symposium at **UTMB, Galveston, TX** (**2008**)
19. **J. W. Craft, Jr**. and G. B. Legge, The Role of Entropic Priming of the LFA-1 I-domain in High Affinity ICAM Binding, 12th Annual Sealy Structure Biology Symposium at **UTMB, Galveston, TX** (**2007**)
20. **J. W. Craft, Jr**., R. Carreno, M. Sen, and G. B. Legge , Mechanistic and Structural Insights into the Activation of the LFA-1 I-domain, 20th Annual Symposium of the Protein Society, San Diego, CA (**2006**)
21. **J. W. Craft, Jr**., Y. Xia, G. B. Legge, Probing LFA-1 I-domain Spectra Enhanced by New Cryo Probe, 11th Annual Sealy Structure Biology Symposium at UTMB (**2006**)
22. **J. W. Craft, Jr**., G. B. Legge, Probing LFA-1 I-domain Spectra Enhanced by New Cryo Probe, Sigma Xi, Houston, TX (**2006**)
23. **J. W. Craft, Jr**. and G. B. Legge, An AMBER/DYANA/MOLMOL Phosphorylated Amino Acid Library Set And Incorporation into NMR Structure Calculations, 10th Annual Sealy Structure Biology Symposium at UTMB, Galveston, TX (**2005**)
24. **J. W. Craft, Jr**. and G. B. Legge, An AMBER/DYANA/MOLMOL Phosphorylated Amino Acid Library Set And Incorporation into NMR Structure Calculations, Sigma Xi, Houston, TX (**2005**)

FUNCTIONS AND SIMULATION ENVIRONMENTS

Principle Function Owner for **Space Shuttle** Control Systems
Ascent Digital Auto Pilot (DAP), Ascent First Stage Guidance, Ascent Second Stage Guidance
Return to Launch Site (RTLS) Guidance, Contingency Guidance
Manager and Developer for Shuttle Simulations
Shuttle Engineering Simulation (SES and X38)
Shuttle Trajectory & Mission Planning Simulation (STAMPS), Flexible Airframe Response (FAR)
Developer in Fortran, C, **C++**, Ada, R, MatrixX, and **Matlab**
Developer in Perl, **Python**, Java, PySpark,
Configuration Control Administrator in Clear Case, GITHUB
Manager and Developer for Big Data Simulations
GROMACS, LAMMPS, AMBER, NAMD,
PolyFTS; GAUSSIAN-QM; FIREFLY-QM, **TENSOR FLOW,** NVIDIA

MENTORING OF STUDENTS LEADING TO SUCCESS

Students / Collaboration mentored (38)
(SURF: Summer Undergraduate Research Fellowship; PURS: Provost Undergraduate Research Scholarship; Goldwater: Barry Goldwater Scholarship; CURE: Cardiovascular Undergraduate Research Experience)

Eliason Lewis (2026-2027)	PURS candidate
Catherine Ly-ha (2026-2028)	PURS candidate
Ruba Al-Showaiter (2026-2028)	SURF candidate
Angela Vu (2026)	Public Health Intern
Anuj Kurella (2025-2026)	SURF
Caleb Chiao (2025)	UH-CURE
Justin Griffin (2024-2026)	**Griffin Labs LLC**
Ashlynn Armour (2024)	UH-CURE
Tasneem Islam (2021-22) SURF,PURS	UH plan 2023
Elizabeth Merlinsky (2018-20) SURF, PURS	**JAMP-Baylor MED School**
Luis Cavazos (2019-20) PURS	UH (2022) **Lakeside MRI**
Ashley Cruz (2019-20)	**Fulbright ETA/PA UTMB**
Kinal Patel (2019-20) SURF, PURS	**John's Hopkins; Grad School**
Karim Matta (2020)	UH (2020) **Mast BioMed Diagnosics ASU**

Sashank Shorey (2018-20) SURF, Honors Thesis **Baylor MED School**
Big Data for Drug Discovery in the Cloud

Safa Ali (2018-19) **Medical Assistant at AFC Urgent Care**
Targeting Borrelia burgdorferi Proteins in Lyme Disease UH (2019)

Sonakshee Shree (2018-19) TBD
Cholera Disease UH (post BA)

Amir Nazarian (2017-18) PURS **South Texas College of Law**
Large Scale Docking of Chemical Compounds Against CDK20 UH (2018)

Aresh Bial (2018) PURS UH (2018)
Molecular Dynamics Energy Landscapes for Rho Associated Kinase Activation Loop

Andrew Gula (2017-18) **UQ Ochsner Au/New Orleans**
Search for Allosteric Inhibitors for Rho Associated Kinase

Asra Aslam (2017-18) PURS **UT Med San Antonio**
Computational Screening for Small Molecule Inhibitors of Talin/B3 Integrin Tail

Farhan Mithani (2016) Honors Thesis **MD stud Texas AM, College Station**
Complex Interface between Tissue Factor Cytoplasmic Tail and the Pin-1 WW Domain

Stefanny Ortega (2016) **Pharmacy Technician**

Nadia Naghi (2016) **Health Advancing Together**

Oladipo Soetan (2016) **MD American U Antigua Med**

Amir Ali (2013-15) SURF, PURS **MD UTMB Galveston**

Molecular Dynamics Analysis of a Monte Carlo for Pin1 WW domain/TFCD Complex

Lindsey Brier (2012-14) Honors Thesis; PURS, Goldwater **MD/PhD WashU, St.Lious**
Differential Toxicity of Cholera Toxin and Enterotoxin Explored Using MD Sims

Jeff Mindrebo (2011-13) Honors Thesis; SURF **Ph.D UC San Diego**
Computational Docking and Analysis of a Peptide Linked Inhibitor of Rho Associated Kinase

Tangen Tran (2010-12) Honors Thesis; Work Study
Computational pKa Analysis of ROCK with Cofactors and Phosphorylated Residues

Chris Britt (2011) Summer Student
Inhibition of Cholera Toxin and Other AB Toxins by Polyphenolic Compounds

Kim Ngo (2010)

Ksenia Ivaschuk (2010) SURF, Work Study

Archana Shah (2009-10) SURF **MD 2015 Texas Tech U Health**
Drug Discovery for Inhibition of ROCK1 in Cardiac Fibrosis **Science Center**

Pamela Mbonu (2009)

Mark Herzik (2008) Honors Thesis; **Ph.D 2014 UC Berkeley/Postdoc Scripps San Diego**
Phosphate-dependent Ligand Affinity Switching within the Tissue Factor Cytoplasmic Domain

MENTORING PUBLICATIONS

PUBLICATIONS IN REFEREED JOURNALS

1. D Bakthavatsalam, J.W. Craft Jr., A Kazansky, N Nguyen, G Bae, A.R. Caivano1, C.W. Gundlach IV, **A Aslam, S Ali**, S Gupta, S.Y. Lin, H.D. Parthiban, P Vanderslice, C.C. Stephan and D.G. Woodside; Identification of Inhibitors of Integrin Cytoplasmic Domain Interactions With Syk; Front. Immunol., 08 January (**2021**) 10.3389/fimmu.2020.575085
2. **Reza Abbasgholizadeh**, Hua Zhang, J.W. Craft Jr, Robert M Bryan Jr, Steven J Bark, James M Briggs, Robert O Fox, Anton Agarkov, Warren E Zimmer, Scott R Gilbertson, Robert J Schwartz. Discovery of vascular Rho kinase (ROCK) inhibitory peptides. (**2019**) PMID: 31132884 PMCID: PMC6690139 DOI: 10.1177/1535370219849581
3. P Cherubin, MC Garcia, D Curtis, **CB Britt**, J.W. Craft Jr., H Burress, C Berndt, S Reddy, J Guyette, T Zheng, Q Huo, B Quiñones, JM Briggs, K Teter. Inhibition of Cholera Toxin and Other AB Toxins by Polyphenolic Compounds. PLoS One. Nov 9;11(11), (**2016**)
4. J.W. Craft Jr., T. Shen, **L. M. Brier**, and J. M. Briggs. Biophysical Characteristics of Cholera Toxin and Escherichia coli Heatlabile Enterotoxin Structure and Chemistry Lead to Differential Toxicity. J Phys Chem B, (**2015**).
5. J.W. Craft Jr., H. Zhang, M. N. Charendoff, **J. T. Mindrebo**, R. J. Schwartz, J. M. Briggs. Associations between the Rho kinase-1 catalytic and PH domain regulatory unit. J Mol Graphic Model, 46: 74-82 (**2013**).
6. M. Sen, **M. Herzik**, J.W. Craft Jr., A.L. Creath, S. Agrawal, W. Ruf, and G. B. Legge. Spectroscopic characterization of successive phosphorylation of the tissue factor cytoplasmic region. Open Spec J, 3:58-64 (**2009**)

STUDENTS WITH SENIOR HONORS THESIS

1. **Farhan Mithani**, COMPUTATIONAL ANALYSIS OF PEPTIDYL-PROLYL ISOMERASE PIN1 AND TISSUE FACTOR CYTOPLASMIC DOMAIN; Fall (2016)
2. **Lindsey Brier**, EXPLORING THE CAUSES OF DIFFERENTIAL TOXICITY BETWEEN CHOLERA TOXIN AND ENTEROTOXIN USING MOLECULAR DYNAMICS SIMULATIONS, Spring (2014)
3. **Jeff Mindrebo**, COMPUTATIONAL MODELING, DOCKING, AND SIMULATION OF BIVALENT INHIBITORS FOR RHO ASSOCIATED KINASE, Fall (2013)
4. **Tangen Tran**, COMPUTATIONAL PKA ANALYSIS OF ROCK WITH COFACTORS AND PHOSPHORYLATED RESIDUES; Spring (2013)

NATIONAL SCHOLARSHIPS

1. **Ashley Cruz, Fulbright ETA Fellowship Program**, International program to sponsor her as a mentor for students at Instituto Tecnologico Superior de Zacapoaxtla, Zacapoactla Mexico; (2021)
2. **Lindsey Brier, Barry Goldwater Scholarship**, A nationally recognized scholarship for students to pursue research career in the natural sciences; (2013)

MENTORED PROCEEDINGS AND POSTERS

1. **Caleb Chiao,** Darren G. Woodside, John W. Craft Jr.; Using Molecular Dynamics Simulation to Discover Inhibitors of Talin to Integrin Binding; American Heart Association Basic Cardiovascular Sciences Scientific Sessions July 22st – Jul 26th, (**2025**) Baltimore, MD
2. **Ashlynn Armour,** Ron Biediger, Darren G. Woodside, John W. Craft Jr.; Analyzing the Chemical Features of Lead Compounds for the Inhibition of SYK Signaling; American Heart Association Basic Cardiovascular Sciences Scientific Sessions July 21st – Jul 25th, (**2024**) Chicago, IL
3. **Luis Cavazos**, **Zain Hussain**, Ronald Biediger, David Maxwell, Peter Vanderslice, Darren Wodside, and John W. Craft Jr; Trajectories and Comparative Analysis of Compounds that Bind α4β1 and α4β7 (**2020**)
4. **Elizabeth A. Merlinsky**, **Sashank Shorey**, **Safa Ali**, Steven J. Bark, Ron Biediger, Robert J. Schwartz, Bradley K. McConnell, Darren G. Woodside, John W. Craft Jr.; Cloud Computing for Drug Discovery: Workflow and Implementation in Targeting Spleen Tyrosine Kinase/SYK (**2020**) PURS
5. **Karim Matta**, **Ashley Cruz**, John W. Craft, Jr.; Computational Analysis of 1XTC and Mutant 1XTC (D229E) (**2020**)
6. **Kinal Patel**, Brad McConnell, Robert Schwartz, John Craft Jr.; The SRF/NKX 2.5 Regulatory Node (**2020**)
7. **Amir Nazarian**, Xin Wang, Fang Yu, Yu Liu and John W. Craft, Jr., Large Scale Docking of Chemical Compounds Against CDK20; UH Undergraduate Poster Session Oct 12 (2017) PURS
8. **Andrew Gula**, Robert J. Schwartz and John W. Craft, Jr., The Search for Allosteric Inhibitors for Rho Associated Kinase; UH Undergraduate Poster Session Oct 12, (2017) PURS
9. **Asra Aslam**, Darren Woodside, Robert J. Schwartz and John W. Craft, Jr.; Computational Screening for Small Molecule Inhibitors of Talin/B3 Integrin Tail Interactions; UH Undergraduate Poster Session Oct 12, (2017) PURS
10. **Amir Ali**, John W. Craft Jr., and, James M. Briggs; Molecular Dynamics Simulations of Tissue Factor Cytoplasmic Region/Pin1-WW Domain Complex; Sealy Center for Structural Biology Symposium, (2015) Galveston SURF, PURS

11. **Amir Ali**, John W. Craft Jr., and, James M. Briggs; Molecular Dynamics Simulations and Analysis of a Monte Carlo for Pin1 WW domain/TFCD Complex; UH Research Day (2014)
12. **Lindsey Brier**, John Craft Jr., Tsai-wei Shen, and James Briggs; Differential Toxicity of Cholera Toxin and Enterotoxin Explored Using MD Simulations; **National Council on Undergraduate Research**, University of **Kentucky** (2014) PURS
13. **Lindsey Brier**, John Craft Jr., Tsai-wei Shen, and James Briggs; Differential Toxicity of Cholera Toxin and Enterotoxin Explored Using Molecular Dynamics Simulations; 18th Annual Sealy Structural Biology Symposium (2014) Galveston
14. **Jeff Mindrebo**, John W. Craft Jr., Hua Zhang Robert J. Schwartz and, James M. Briggs; Computational Docking and Analysis of a Peptide Linked Inhibitor of Rho Associated Kinase; 18th Sealy Structural Biology Symposium, (2013) Galveston
15. **Jeff Mindrebo**, John W. Craft Jr., Hua Zhang Robert J. Schwartz and, James M. Briggs; Computational Docking and Analysis of a Peptide Linked Inhibitor of Rho Associated Kinase; **Texas Undergraduate Research Day at the Capitol**, (2013) Austin
16. **Jeff Mindrebo**, John W. Craft Jr., Hua Zhang Robert J. Schwartz and, James M. Briggs; Computational Docking and Analysis of a Peptide Linked Inhibitor of Rho Associated Kinase; UH Undergraduate Poster Session, (2012) SURF
17. **Jeff Mindrebo**, John W. Craft Jr., Hua Zhang Robert J. Schwartz and, James M. Briggs; Computational Docking and Analysis of a Peptide Linked Inhibitor of Rho Associated Kinase; 22nd KECK Symposium, (2012)
18. **Tangen Tran**, John W. Craft Jr., Robert J. Schwartz and, James M. Briggs; pKa and Electrostatic Analysis of ROCK1 Catalytic Domain; Sealy Center for Structural Biology Symposium (2012)
19. **Tangen Tran**, John W. Craft Jr., Robert J. Schwartz and, James M. Briggs; pKa and Electrostatic Analysis of ROCK1 Catalytic Domain; UH Spring Research Symposium, (2012)
20. **Archana Shah**, John W. Craft Jr., Hua Zhang Tsaiwei Shen, Robert J. Schwartz and, James M. Briggs; Drug Discovery for Inhibition of ROCK1 in Cardiac Fibrosis; UH Undergraduate Poster Session, (2010) SURF

ADDITION WORK MATERIALS

OTHER GRANTS SUBMITTED but NOT FUNDED

1. Novel Rho Kinase Inhibitor Therapy for Cardiovascular Disease, American Heart Association, PI Craft/Mentor Dr. Schwartz
2. ROCK Catalytic and PH Domain Activation Mechanisms in Cardiovascular Disease, American Heart Association, PI Craft/Mentor Dr. Schwartz
3. Allostery and Energy Landscapes in Integrin Activation, NIH F32 Fellowship Application, PI Craft/Mentor Dr. Briggs
4. NanoVelcro: Leukocyte Function Associated antigen-1 Directed Uptake of Particles, Alliance for NanoHealth Fellowship, PI Craft/Mentor Dr. Briggs
5. Allostery and Energy Landscapes of Integrin Activation Key to Pharmacophore Models and Drug Design, Texas Advanced Research Program pre-proposal, PI Dr. Briggs/Senior Person Craft
6. LFA-1 Activation: A Pathway for Inhibitor Lead Generation Against Arthritis, Arthritis Foundation, PI Craft/Mentor Dr. Briggs/Co-mentor Dr. Sandeep Agarwal
7. Designing Macromolecular Integrin-Nanoparticles with Receptor Specific Adhesion Characteristics, NSF Macromolecular, Supramolecular and Nanochemistry, PI Dr. Briggs /Co-PI Dr. Mauro Ferrari/Senior Person Craft

INTERNAL TECHNICAL PAPERS

Shuttle SRB TVC Rate and Deflection Requirement Analysis

MAJOR TECHNICAL BRIEFINGS; sample highlights among many

SMART Development Task, June 11 (2002)
Autonomous Planning and Optimal GN&C Enabling Effort (APOGEE) June 10 (2002)
Abort Risks During RTLS ET Separation and Comparisons to TAL ET Debris Hit Probability, PRCB, May 22 (2002)
Cross Cutting Technologies Between Shuttle 2020 and SLI, May 17 (2002) Next Steps in ABORT Safety Enhancements, March 27 (2002)
Why Autonomous Flight Management? Why Now?!, March 4 (2002) Abort Performance Enhancements Certification Approach (2001)
Integration of Change for RCS Window Protection Iload Change, SASCB, Feb 26 (2001)
Statistical Treatment of BSM Firing Data For Requirements Verification, Sep 7 (2000)
Performance Enhancement Critical Design Review (CDR) GN&C Representative
SRB TVC Requirements Briefing
Flight Readiness Review (FRR) for STS-93 Flight Control Redesign Phased Performance Enhancement Implementation for payload Chandra X-Ray Telescope (1999)
Multiple Performance Enhancement Briefings, PRCB's, and FRR's

TECHNICAL SEMINARS

Co-developer of the Biophysics Curriculum at UH (2007)
Monte Carlo Training [For SESII and Matlab] NASA Johnson Space Center, (regular)
Design of Experiments Instructor, NASA Johnson Space Center (regular)
Clear Case User Training Instructor, NASA Johnson Space Center (regular)

PROFESSIONAL ACTIVITIES

PROFESSIONAL MEMBERSHIPS

American Institute of Aeronautics and Astronautics (AIAA)
American Heart Association (AHA)
American Society for Pharmacology and Experimental Therapeutics (ASPET)
Protein Society

ADDITION WORK EXPERIENCE

B & D Avionics, Industrial Engineer, Wichita, KS, 1989 - 1989
Developed a Mil-Spec and Montreal CFC treaty compliant process for the final cleaning and closeout of circuit board production for aircraft instruments. Responsible for the research of vendors used in a cockpit voice recorder development project.

Learjet, Engineering Technical Assistant, Wichita, KS, 1988 - 1988
Part of the flight test team for the Lear Model 31 and 55C, including data reduction and analysis. The correlation of bleed flow between the engines of the two test aircraft enabled climb performance data to be compiled for FAA certification.

FUNCTIONS AND SIMULATION ENVIRONMENTS

Principle Function Owner for Space Shuttle Control Systems
Ascent Digital Auto Pilot (DAP) Ascent First Stage Guidance Ascent Second Stage Guidance
Return to Launch Site (RTLS) Guidance Contingency Guidance
Manager and Developer for Shuttle Simulations
Shuttle Engineering Simulation (SES)

Shuttle Trajectory and Mission Planning Simulation (STAMPS) Flexible Airframe Response (FAR)
Developer in Fortran, C, C++, Ada, R, MatrixX, and Matlab
Developer in Perl, Python, Java, PySpark,
Configuration Control Administrator in Clear Case, GITHUB
Manager and Developer for Big Data Simulations
GROMACS, LAMMPS, AMBER, NAMD,
GAUSSIAN-QM; FIREFLY-QM, TENSOR FLOW