

EDUCATIONAL BACKGROUND

- 2014.** Doctor of Philosophy in Physics, University of Southern California (USC), USA.
- 2012.** Master of Computer Science in High Performance Parallel Computing & Simulations, USC, USA. (Dual Program with PhD Degree in Physics).
- 2005.** Bachelor of Science in Physics, Honors Program, Hanoi National University of Education, Vietnam.
- 2001.** Ha-Long Highschool for Gifted Students, Quang Ninh, Vietnam.

RESEARCH POSITIONS

- 2021-Now.** **Computational Biophysicist (Staff)**, Advanced Computing for Life Sciences and Engineering Group, Science Engagement Section, Computing and Computational Sciences, Oak Ridge National Lab, TN, USA.
- 2018-21.** **Director's Postdoctoral Fellow**, Center of Nonlinear Studies, Los Alamos National Lab (LANL), NM, USA. Supervisor: Dr. Angel E. Garcia (the Center's Director).
- 2014-18.** **CIHR and AIHS Postdoctoral Fellow** at the Institute of Biocomplexity & Informatics, Department of Biological Sciences, University of Calgary, Canada. Supervisor: Prof. Dr. Sergei Noskov, Associate Head of Research.
- 2011-14.** **Research Assistant** in Computational Condensed Matter Theory Group, Department of Physics, University of Southern California (USC), USA. Advisors: Prof. Dr. Stephan Haas and Prof. Dr. Robert Farley.
- 2008-11.** **Research Assistant** at Collaboratory for Advanced Computing and Simulations, Department of Physics, USC, USA.

COMPETITIVE HONORS AND AWARDS/GRANTS

- 2018-21.** LANL Director's Fellow, Project Title: "*Molecular Basis of RAS-related Cancers*". Award \$89,700/year.
- 2016-18.** Canadian Institutes of Health Research (CIHR) Postdoctoral Fellowship, Project Title: "*Drug and pH effects on Ion Selectivity in Sodium and Calcium Channels Underlying Arrhythmias*." Award \$90,000 Canada.
- 2015-17.** Alberta Innovates-Health Solutions (AIHS) Postdoctoral Fellowship, Project Title "*Drug and pH Regulations of Ion Permeability in Sodium and Potassium Channels: Molecular Basis of Cardiac Dysrhythmias*." Award \$165,000 Canada.
- 2016.** Ed McCauley Postdoctoral Award for Excellent Research (\$1,000), Department of Biological Sciences, University of Calgary, AB, Canada.

COMPUTING AWARDS

- 2024.** INCITE Allocation, Co-PI with Dr. Lei Shi, NIH. Project Title "*Mechanism of β -arrestin Activation*".
- 2021-24.** Anton2 Allocations, Co-PI with Dr. Thomas Szyperski (University of Buffalo). Project Title "*Protein Core Water Penetration at the Onset of Cold Denaturation*".

RESEARCH INTERESTS

Research topics include, but not limited to, ion channels, Ras-related cancer, Raf, Arrestin, drug design, lipid-drug interactions, radio-isotopes, molecular dynamics simulations, free-energy calculations, non-equilibrium/enhanced sampling, force field developments, Markov State Modeling and machine learning/artificial intelligence (ML/AI) applied to life sciences. One of my goals is to find clinically efficient

noncovalent drugs for targeting cancer cells and mutant signaling proteins including GTPases such as Ras, Raf kinases, and Arrestin, and related protein-protein interactions networks at both atomic details and microscopic scales.

COLLABORATORS

Drs. Tom Beck, Jens Glaser, Dilip Asthagiri, David Rogers, Debsindhu Bhowmik, Anuj Kapadia, Sandra Davern, Thomas Szyperski, Angel Garcia, David Hoogerheide, Tatiana Rostovtseva, David Hardy, Paolo Carloni, Edward Lyman, Lei Shi, Jonathan Javitch, Peter Tieleman.

PEER-REVIEWED PUBLICATIONS (31)

<https://scholar.google.ca/citations?user=8HrtAJUAAAAJ&hl=en>

1. **2024. Van A. Ngo.** *Insight into Molecular Basis and Dynamics of Full-length CRAf Kinase in Cellular Signaling Mechanism.* DOI:10.1016/j.bpj.2024.06.028. Data:10.13139/OLCF/2396898.
2. **2024.** Miranda N Limbach, Edward T Lindberg, Hernando J Olivos, Lara van Tetering, Carlos A Steren, Jonathan Martens, **Van A. Ngo**, Jos Oomens, Thanh D Do. *Taming Conformational Heterogeneity on Ion Racetrack to Unveil Principles that Drive Membrane Permeation of Cyclosporines.* DOI: 10.1021/jacsau.4c00011.
3. **2024.** Yibo Wang, **Van A. Ngo**, Xiaohui Wang. Stereoselective recognition of morphine enantiomers by μ -opioid receptor. DOI: 10.1093/nsr/nwae029.
4. **2023. Van A. Ngo**, Yen Ting Lin, and Danny Perez, *Improving Estimation of the Koopman Operator with Kolmogorov–Smirnov Indicator Functions.* J. Chem. Theory Comp. DOI: 10.1021/acs.jctc.3c00632.
5. **2022.** Meruyert Kudaibergenova, Jiqing Guo, Hanif M Khan, James Lees-Miller, Mahdi Mousaei, Williams Miranda, **Van A. Ngo**, Sergei Yu Noskov, D Peter Tieleman, Henry J Duff. *The Voltage-Sensing Domain of a hERG1 Mutant is a Cation-selective Channel.* Biophysical Journal. DOI: 10.1016/j.bpj.2022.10.032.
6. **2022. Van A. Ngo**, Maria Queralt-Martin, Farha Khan, Lucie Bergdoll, Jeff Abramson, Sergey M. Bezrukov, Tatiana K. Rostovtseva, David P. Hoogerheide, and Sergei Yu. Noskov. *The Single Residue K12 Governs the Exceptional Voltage Sensitivity of Mitochondrial Voltage-Dependent Anion Channel Gating.* JACS. DOI: 10.1021/jacs.2c03316.
7. **2022. Van A. Ngo** and Angel E. Garcia, *Millisecond molecular dynamics simulations of KRas-dimer formation and interfaces.* Biophysical Journal. DOI: 10.1016/j.bpj.2022.04.026. Blogpost: <https://www.biophysics.org/blog/hydrolyzable-kras-dimer-1>. (Cover Article)
8. **2021. Van A. Ngo** and Ramesh K. Jha, *Identifying key determinants and dynamics of SARS-CoV-2/ACE2 tight interaction*, PlosOne, DOI: 10.1371/journal.pone.0257905.
9. **2021.** Kevin R. DeMarco, ..., **Van A. Ngo**, ..., Colleen E. Clancy and Igor Vorobyov. *Molecular determinants of pro-arrhythmia proclivity of d-and l-sotalol via a multi-scale modeling pipeline.* J. Molecular and Cellular Cardiology. DOI: 10.1016/j.yjmcc.2021.05.015
10. **2021. Van A. Ngo**, Hui Li, Toby Allen, Alexander Mackerell, Benoit Roux, and Sergei Noskov, *“Polarization Effects of Water on Selective Cation Transport Across a Narrow Transmembrane Channel”*, J. Chem. Theory Comp. DOI: 10.1021/acs.jctc.0c00968.
11. **2020. Van A. Ngo**, Sumantra Sarkar, Chris Neale, and Angel E Garcia. *How Anionic Lipids Affect Spatiotemporal Properties of KRAS4B on Model Membranes.* J. Phys. Chem. B 2020. DOI: 10.1021/acs.jpcb.0c02642. (Cover Article)
12. **2020.** Yingying Zhang, Kamran Haider, Divya Kaur, **Van A. Ngo**, Xiuhong Cai, Junjun Mao, Umesh Khaniya, Xuyu Zhu, Sergei Noskov, Themis Lazaridis, M.R. Gunner. *Characterizing the water wire in the gramicidin channel found by Monte Carlo sampling using continuum electrostatics and in Molecular Dynamics trajectories with conventional or polarizable force fields.* J. of Theo. and Comp. Chem. DOI: 10.1142/S0219633620420018
13. **2019.** Trung Hai Nguyen, **Van A Ngo**, João Paulo Castro Zerba, Sergei Noskov, and David DL Minh, *Nonequilibrium path-ensemble averages for symmetric protocols*, J. Chem. Phys. 151, 194103 (2019). DOI: 10.1063/1.5121306.

14. 2019. Yibo Wang, Rocio Finol-Urdaneta, **Van A. Ngo**, Sergei Noskov, and Robert French, *Bases of Bacterial Sodium Channel Selectivity Among Organic Cations*, Scientific Reports. DOI: doi.org/10.1038/s41598-019-51605-y.
15. 2019. **Van A. Ngo**, John Keenan Fanning and Sergei Yu. Noskov. *Comparative Analysis of Protein Hydration from MD simulations with Additive and Polarizable Force Fields*, Advanced Theory and Simulations (Wiley), DOI: doi.org/10.1002/adts.201800106.
16. 2018, Williams Ernesto Miranda, **Van A. Ngo**, Ruiwu Wang, Lin Zhang, SR Wayne Chen, Sergei Yu Noskov, *Molecular Mechanism of Conductance Enhancement in Narrow Cation Selective Membrane Channels*, J. Phys. Chem. Lett., DOI: 10.1021/acs.jpclett.8b01005.
17. 2017. Williams Ernesto Miranda, **Van A. Ngo**, Laura L Perissinotti, and Sergei Y. Noskov, *Computational Membrane Biophysics: Connecting Ion Channels-Ligand Interactions to Cellular Function and Pharmacology*, BBA -Proteins and Proteomics, DOI: 10.1016/j.bbapap.2017.08.008. (Co-first authors)
18. 2017. Hristina Zhekova, **Van A. Ngo**, Mauricio C. da Silva, Dennis Salahub, and Sergei Noskov, *Selective Ion Binding and Transport by Membrane Proteins – A Computational Perspective*, Coord. Chem. Rev. DOI: 10.1016/j.ccr.2017.03.019.
19. 2017. **Van A. Ngo**, Laura L Perissinotti, Williams Ernesto Miranda, Wayne Chen, and Sergei Noskov, *Mapping Ryanodine Binding Sites in the Pore Cavity of Ryanodine Receptor*, Biophys. J., DOI: 10.1016/j.bpj.2017.03.014
20. 2016. Williams Ernesto Miranda, **Van A. Ngo**, Pedro Alberto Valiente, and Sergei Yu. Noskov, *Improved QM/MM Linear Interaction Energy Model for Substrate Recognition in Zinc-Containing Metalloenzymes*, J. Phys. Chem. B, DOI: 10.1021/acs.jpcb.6b05628.
21. 2016. **Van A. Ngo**, Yibo Wang, Stephan Haas, Sergei Noskov, and Robert Farley, *K⁺ Block Is the Mechanism of Functional Asymmetry in Bacterial Nav Channels*, PLoS Comput Biol 12(1): e1004482. doi:10.1371/journal.pcbi.1004482.
22. 2016. **Van A. Ngo**, Ilsoo Kim, Toby Allen, and Sergei Noskov, *Estimation of Potentials of Mean Force from Non-Equilibrium Pulling Simulations Using both Minh-Adib Estimator and Weighted Histogram Analysis Method*, J. Chem. Theory Comp. DOI: 10.1021/acs.jctc.5b01050.
23. 2015. **Van A. Ngo**, Mauricio C. da Silva, Maximilian Kubillus, Hui Li, Benoît Roux, Marcus Elstner, Qiang Cui, Dennis R. Salahub and Sergei Noskov, *Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins*, J. Chem. Theory Comp. DOI: 10.1021/acs.jctc.5b00524.
24. 2015. Dennis R. Salahub, Sergei Yu. Noskov, Bogdan Lev, Rui Zhang, **Van A. Ngo**, Annick Goursot, Patrizia Calaminici, Andreas M. Köster, Aurelio Alvarez Ibarra, Daniel Mejía Rodríguez, Jan Řezáč, Fabien Cailliez and Aurélien de la Lande, *Review: QM/MM Calculations with deMon2k*, Molecules 2015, 20(3), 4780-4812; doi:10.3390/molecules20034780.
25. 2015. Hui Li*, **Van A. Ngo***, Mauricio Silva*, Dennis R. Salahub, Sergei Noskov and Benoît Roux. "Representation of Ion-Protein Interactions using the Drude Polarizable Force-Field", J. Phys. Chem. B, 2015, 119 (29), pp 9401–9416. (Co-first Authors).
26. 2014. **Van A. Ngo**, Rosa Di Felice and Stephan Haas, "Is The G-quadruplex an Effective Nanoconductor for Ions?", J. Phys. Chem. B, 2014, 118 (4), pp 864–872 DOI: 10.1021/jp408071h.
27. 2014. **Van A. Ngo**, Darko Stefanovski, Stephan Haas and Robert Farley, "Non-Equilibrium Dynamics Contribute to Ion Selectivity in The KcsA Channel". PLoS ONE 9(1): e86079. DOI:10.1371/journal.pone.0086079.
28. 2012. **Van A. Ngo** and Stephan Haas, "Demonstration of Jarzynski's Equality in Open Quantum Systems Using a Step-wise Pulling Protocol", Phys. Rev. E 86, 031127 (2012).
29. 2012. **Van A. Ngo**, Rajiv Kalia, Aiichiro Nakano, and Priya Vashishta, "Molecular Mechanism of Flip-flop in Triple-layer Oleic-Acid Membrane: Correlation Between Oleic Acid and Water", J. Phys. Chem. B, 2012, 116 (45), pp 13416–13423.
30. 2012. **Van A. Ngo**, Rajiv Kalia, Aiichiro Nakano, and Priya Vashishta, "Supercrystals of DNA-functionalized Gold Nanoparticles: A Million-Atom Molecular Dynamics Simulation Study", J. Phys.

Chem. C, **2012**, 116 (36), pp 19579–19585.

31. **2012. Van A. Ngo**, “Parallel-pulling Protocol for Free-Energy Evaluation”. Phys. Rev. E **85**, 036702 (2012).

INVITED/CONFERENCE TALKS/POSTERS (19)

1. **2024. Van A. Ngo** and Lei Shi, *Towards Revealing Functionally Relevant Conformational Dynamics of β -Arrestins*. Biophysiscal Society.
2. **2023. Van A. Ngo**. *Insights into Molecular Basis of Cellular Signaling Pathways*. CECAM 2023. Pisa Italy.
3. **2022. Van A. Ngo**. *Insights into KRas Dimerization and Potential for GTP Hydrolysis via Ras Dimer*. Calgary, Canadian Chemistry Conference 2022.
4. **2021. Van A. Ngo***, and Angel E. Garcia, *Revealing the Dynamics of KRAS4B Dimerization on Anionic Membrane from One Millisecond all Atom Molecular Dynamics Simulations*. Biophysical Journal 120 (3), 288a.
5. **2021. Van A. Ngo**, *Insights into Cellular Signaling Mechanisms of KRas Monomer and Dimer on Lipid Membranes via Newton Dynamics*, Colloquium at Department of Physics, Oakland University.
6. **2020. Van Ngo** and Angel Garcia, “*Insights into the Dynamics of RAS on Lipid Membranes for Understanding Cellular Signaling*”, American Chemical Society (Online) Symposium. DOI: 10.1021/scimeetings.0c06984
7. **2020. Van Ngo**, “*Insights into the Dynamics of RAS on Lipid Membranes for Understanding Cellular Signaling*”, Colloquium at Department of Physics, University of Texas-Dallas.
8. **2019. Van Ngo**, “*Molecular Dynamics Simulations: An Atomic-Resolution Microscope to Unravel Molecular Mechanisms of Biological Systems*”, a Colloquium at Department of Physics, Wayne State University, USA.
9. **2018. Van Ngo**, “*Molecular Dynamics Simulations: Unravelling Conformational Changes and Kinetics of Proteins*”, at McGill University (hosted by Prof. Huy Bui) and University of Montreal (hosted by Prof. Rikard Blunck), Canada.
10. **2017. Van Ngo**, “*From Ion Selectivity to Drug Design in Transmembrane Proteins*”, Center for Nonlinear Studies, Los Alamos National Lab. USA.
11. **2017. Van Ngo**, Williams Miranda, Laura Perissinotti, Wayne SR Chen, Sergei Noskov, “*Understanding the Binding Mechanism of Ryanodine to the Open-and Closed States of the Ryanodine Receptor Pore*”, Biophysical Society Conference. USA.
12. **2016. Van Ngo**, “*Frontiers in Studies of Interactions and Functionalities of Ion-Protein Complexes by Molecular Dynamics Simulations*”, Winner Presentation of 2016 Ed McCauley Postdoctoral Award at Biological Students Symposium, Dept. of Biological Sciences, University of Calgary. Canada.
13. **2016. Van Ngo**, “*DeMon developers workshop*”, Henan University of Technology, Zhengzhou, P.R., China 450001.
14. **2016. Van Ngo** and Sergei Noskov, “*A Trio of Cations in Gramicidin a Channel: Importance of Quantum Effects to Describe Ion Selectivity of K⁺ and Na⁺, and Proton Transfer*”, Biophysical Society. USA.
15. **2016. Van Ngo**, “*String Method*”, 7th Kananaskis Symposium on Molecular Dynamics Simulations. Canada.
16. **2015. Van Ngo**, “*Computation of Convergent Free Energy Profiles from Non-equilibrium Pulling Simulations*”, 6th Kananaskis Symposium on Molecular Dynamics Simulations. Canada.
17. **2014. Van Ngo**, Bogdan Lev, and Sergei Noskov, “*Hands-on Trainings for Quantum Mechanics and Molecular Mechanics (QM/MM) Simulations*”, 2nd Molecular Simulation Summer School, Centre for Molecular Simulation, University of Calgary. Canada.
18. **2013. Van Ngo**, “*Jarzynski's Equality and Ion Selectivity*”, Department of Biological Sciences, University of Calgary. Canada.
19. **2013. Van Ngo** and Stephan Haas, “*Thermalization Processes in Quantum Mechanics*”, American Physical Society Meeting, USA.

COMPUTING/SCRIPTING SKILLS/LANGUAGES

- Software: NAMD, CHARMM, AMBER, Gromacs, DeMon2k
- Scripting Language: Linux, TCL, Python
- Programming Language: Fortran, C++, OpenMPI, CUDA.
- Codes: <https://gitlab.com/ngoav>

REVIEWER FOR

Nature Communication, PNAS, Biophysical Journal, Physical Reviews, Journal of Physical Chemistry B/C.