

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 EXPERIENCES

- 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*".
- 2021-23.** Anton2 Allocations, Co-PI with Dr. Thomas Szyperski (University of Buffalo). Project Title "*Protein Core Water Penetration at the Onset of Cold Denaturation*".

THESIS

- 2014.** PhD Thesis: "*Step-wise Pulling Protocols for Non-Equilibrium Dynamics*". University of Southern California, ProQuest Dissertations Publishing. 3628257. USA. Publication Number: AAT 3628257; ISBN: 9781321038545.

2005. Undergraduate Thesis: “*Bose-Einstein Condensation in An External Trap*”. Hanoi University of Education, Vietnam.

PEER-REVIEWED PUBLICATIONS (28)

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

1. **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.
2. **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.
3. **2022. Van A. Ngo**, Maria Queralto-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.
4. **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)
5. **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.
6. **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
7. **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.
8. **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.jpcc.0c02642. (Cover Article)
9. **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
10. **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.
11. **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.
12. **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.
13. **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.jpcclett.8b01005.
14. **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)

15. 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.
16. 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
17. 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.jpcc.6b05628.
18. 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.
19. 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.
20. 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.
21. 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.
22. 2015. Hui Li*, **Van A. Ngo***, Mauricio Silva*, Dennis R. Salahub, Sergei Noskov and Benoit 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).
23. 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.
24. 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.
25. 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).
26. 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.
27. 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.
28. 2012. **Van A. Ngo**, “Parallel-pulling Protocol for Free-Energy Evaluation”. *Phys. Rev. E* **85**, 036702 (2012).

INVITED/CONFERENCE TALKS (18)

1. 2023. **Van A. Ngo**. *Insights into Molecular Basis of Cellular Signaling Pathways*. CECAM 2023. Pisa Italy.
2. 2022. **Van A. Ngo**. *Insights into KRas Dimerization and Potential for GTP Hydrolysis via Ras Dimer*. Calgary, Canadian Chemistry Conference 2022.

3. **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.
4. **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.
5. **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
6. **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.
7. **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.
8. **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.
9. **2017. Van Ngo**, "*From Ion Selectivity to Drug Design in Transmembrane Proteins*", Center for Nonlinear Studies, Los Alamos National Lab. USA.
10. **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.
11. **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.
12. **2016. Van Ngo**, "*DeMon developers workshop*", Henan University of Technology, Zhengzhou, P.R., China 450001.
13. **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.
14. **2016. Van Ngo**, "*String Method*", 7th Kananaskis Symposium on Molecular Dynamics Simulations. Canada.
15. **2015. Van Ngo**, "*Computation of Convergent Free Energy Profiles from Non-equilibrium Pulling Simulations*", 6th Kananaskis Symposium on Molecular Dynamics Simulations. Canada.
16. **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.
17. **2013. Van Ngo**, "*Jarzynski's Equality and Ion Selectivity*", Department of Biological Sciences, University of Calgary. Canada.
18. **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.

REVIEWER FOR

Nature Communication, PNAS, Biophysical Journal, PRE, Journal of Physical Chemistry B|C.