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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.

RESEARCH EXPERIENCES

2021-. **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).

- Study biophysical and biochemical properties of RAS GTPase in cascades of cellular signaling and cancer developments; Design non-equilibrium sampling techniques for large protein systems and integrate machine-learning/artificial intelligent techniques to computational biology.

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.

- Investigated biochemical mechanisms of ion selectivity, proton transfer, drug design for potassium, sodium, calcium, and proton channels, which involve in heart diseases (arrhythmias); Developed polarizable force fields (collaborate with Prof. Benoit Roux at University of Chicago) to address more accurate biophysical and biochemical processes in biological systems.

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. Advisor: Prof. Dr. Aiichiro Nakano.

COMPETITIVE HONORS AND AWARDS/GRANTS

2021-22. Anton2 and XSEDE Allocations, Co-PI with Dr. Thomas Szyperski (Buffalo). Project Title "*Protein Core Water Penetration at the Onset of Cold Denaturation*".

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.

THESIS

1. **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.
2. **2005.** Undergraduate Thesis: "*Bose-Einstein Condensation in An External Trap*". Hanoi University of Education, Vietnam.

PEER-REVIEWED PUBLICATIONS (23)

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

1. **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.
2. **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
3. **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.
4. **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*)
5. **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
6. **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.
7. **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.
8. **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.
9. **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.

10. **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**)
11. **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.
12. **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
13. **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.
14. **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.
15. **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.
16. **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.
17. **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.
18. **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**).
19. **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.
20. **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.
21. **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).
22. **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.
23. **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.

24. **2012. Van A. Ngo,** "*Parallel-pulling Protocol for Free-Energy Evaluation*". Phys. Rev. E **85**, 036702 (2012).

INVITED/CONFERENCE TALKS

1. **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.
2. **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.
3. **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
4. **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.
5. **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.
6. **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.
7. **2017. Van Ngo**, "*From Ion Selectivity to Drug Design in Transmembrane Proteins*", Center for Nonlinear Studies, Los Alamos National Lab. USA.
8. **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.
9. **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.
10. **2016. Van Ngo, "***DeMon developers workshop*", Henan University of Technology, Zhengzhou, P.R., China 450001.
11. **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.
12. **2016. Van Ngo**, "*String Method*", 7th Kananaskis Symposium on Molecular Dynamics Simulations. Canada.
13. **2015. Van Ngo**, "*Computation of Convergent Free Energy Profiles from Non-equilibrium Pulling Simulations*", 6th Kananaskis Symposium on Molecular Dynamics Simulations. Canada.
14. **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.

15. **2013. Van Ngo**, ”*Jarzynski's Equality and Ion Selectivity*”, Department of Biological Sciences, University of Calgary. Canada.
16. **2013. Van Ngo** and Stephan Haas**,** “*Thermalization Processes in Quantum Mechanics*”*,* American Physical Society Meeting, USA.