

Hai Minh Nguyen

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EDUCATION

Doctor of Philosophy, Chemistry
Stony Brook University, 2014
Advisor: [Carlos Simmerling](#)

Bachelor of Science, Chemistry
Hanoi University of Science, 2006

COMPUTER SKILLS

Languages:

- Proficient: Python/Cython
- Experience: Javascript, C/C++, FORTRAN

Others:

- GIT, software continuous integration, parallel programming (MPI, multiprocessing)

RELEASED SOFTWARE

Lead developer:

- pytraj (written in Python/Cython): Python API for cpptraj: a data analysis package for biomolecular simulation <https://github.com/Amber-MD/pytraj>
- pymdgx (written in Python/Cython): Python API for mdgx simulation package <https://github.com/Amber-MD/pymdgx>
- nglview (written in Python/Javascript/HTML): Jupyter widget to interactively view molecular structures and trajectories, <https://github.com/arse/nglview>

Contributing:

- AMBER program suite (various languages): biomolecular simulation program, <http://ambermd.org>
- cpptraj (written in C++): Biomolecular simulation trajectory/data analysis, <https://github.com/Amber-MD/cpptraj>
- parmed (written in Python): Parameter/topology editor and molecular simulator, <https://github.com/ParmEd/ParmEd>
- MDAnalysis (written in Python): an object-oriented python toolkit to analyze molecular dynamics trajectories, <http://www.mdanalysis.org/>

EXPERIENCE

Postdoctoral Associate

03/2015-present

Rutgers University, PI: [David A. Case](#)

- Developing PHENIX/AMBER interface for protein refinement with alternative conformation
- Applied new Generalized Born solvation models and a Python-based API for recombining Rosetta and Amber force fields for improving structure prediction and design
- Developing conda-build for AMBER suite

Postdoctoral Associate

11/2014-2/2015

Stony Brook University, PI: [Carlos Simmerling](#)

- Added code and introduced newly optimized Generalized-Born solvation parameters for nucleic acid simulation to AMBER suite program

Research Assistant

2018-2014

Stony Brook University, PI: [Carlos Simmerling](#)

- Developed solvent model for protein and nucleic acid simulations.
- Validated force fields.

PUBLICATIONS

Google Scholar statistics: <http://goo.gl/CpC2zg>

Peer Review

1. **Nguyen, H.**; Prez, A.; Bermeo, S.; Simmerling, C., (2015) Refinement of Generalized Born Implicit Solvation Parameters for Nucleic Acids and Their Complexes with Proteins. *J Chem Theory Comput.*
2. **Nguyen, H.**; Maier, J.; Huang, H; Perrone, V; Simmerling, C., (2014) Folding simulations for proteins with diverse topologies are accessible in days with a physics-based force field and implicit solvent. *Journal of the American Chemical Society.*
3. **Nguyen, H.**; Roe, D. R.; Simmerling, C., (2013) Improved Generalized Born Solvent Model Parameters for Protein Simulations. *Journal of Chemical Theory and Computation*, 9 (4), 2020-2034.
4. Shang, Y., **Nguyen, H.**, Wickstrom, L., Okur, A., and Simmerling, C. (2011) Improving the description of salt bridge strength and geometry in a Generalized Born model, *Journal of Molecular Graphics and Modeling* 29, 676-684.

Software

1. **H. Nguyen**, A. Rose, D. Dotson, M.K. Scherer, ngview v0.5, <http://dx.doi.org/10.5281/zenodo.55409>
2. **H. Nguyen**, D.R. Roe, J. Swails, D.A. Case, (2016) PYTRAJ v1.0.0.dev1: Interactive data analysis for molecular dynamics simulations. <http://dx.doi.org/10.5281/zenodo.44612>
3. D.A. Case, R.M. Betz, W. Botello-Smith, D.S. Cerutti, T.E. Cheatham, III, T.A. Darden, R.E. Duke, T.J. Giese, H. Gohlke, A.W. Goetz, N. Homeyer, S. Izadi, P. Janowski, J. Kaus, A. Kovalenko, T.S. Lee, S. LeGrand, P. Li, C. Lin, T. Luchko, R. Luo, B. Madej, D. Mermelstein, K.M. Merz, G. Monard, **H. Nguyen**, H.T. Nguyen, I. Omelyan, A. Onufriev, D.R. Roe, A. Roitberg, C. Sagui, C.L. Simmerling, J. Swails, R.C. Walker, J. Wang, R.M. Wolf, X. Wu, L. Xiao, D.M. York and P.A. Kollman (2016), AMBER 2016, University of California, San Francisco.
4. A. Case, J.T. Berryman, R.M. Betz, D.S. Cerutti, T.E. Cheatham, III, T.A. Darden, R.E. Duke, T.J. Giese, H. Gohlke, A.W. Goetz, N. Homeyer, S. Izadi, P. Janowski, J. Kaus, A. Kovalenko, T.S. Lee, S. LeGrand, P. Li, T. Luchko, R. Luo, B. Madej, K.M. Merz, G. Monard, P. Needham, **H. Nguyen**, H.T. Nguyen, I. Omelyan, A. Onufriev, D.R. Roe, A. Roitberg, R. Salomon-Ferrer, C.L. Simmerling, W. Smith, J. Swails, R.C. Walker, J. Wang, R.M. Wolf, X. Wu, D.M. York and P.A. Kollman (2015), AMBER 2015, University of California, San Francisco.