

## David Do Le Minh

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## Education

- Ph.D., Physical Chemistry 8/2004-6/2007  
University of California, San Diego  
Thesis Title: Free Energy Reconstruction from Irreversible Single-Molecule Pulling Experiments  
Committee: J. Andrew McCammon (advisor), Judy Kim, Elizabeth Komives, Katja Lindenberg, Jose Onuchic, and Peter Wolynes
- M.S., Chemistry 8/2004-6/2006  
University of California, San Diego
- B.A., Chemistry 8/2000-12/2003  
University of California, Berkeley

## Research Experience

- Postdoctoral Research Associate Starting 11/2011  
Duke University, Durham NC  
Advisor: David Beratan

Research to include:

- Developing and applying free energy calculations to design libraries of small organic molecules with high affinity for targeted proteins
- Developing and applying sampling methods to enhance electron transfer calculations in nucleic acids

- Argonne Scholar/Director's Postdoctoral Fellow 8/2009-9/2011  
Argonne National Laboratory, Argonne IL

- Designed and conducted wide-angle X-ray scattering, isothermal calorimetry, and neutron spin echo experiments to study protein-ligand binding and enzyme catalysis in model systems including adenylate kinase, alcohol dehydrogenase, and calmodulin
- Developed and applied statistical methods to analyze protein-ligand interactions with wide-angle X-ray scattering
- Developed method for using nonequilibrium driven processes as Monte Carlo moves
- Developed algorithms for regenerative Markov chain Monte Carlo simulation
- Derived new optimized estimator for absolute free energies from "replica gas" simulations

Postdoctoral Fellow 8/2007-7/2009  
National Institutes of Health, Bethesda MD  
Advisor: Artur Adib

- Invented statistical estimator to compute path-ensemble averages from bidirectional single-molecule pulling and similar experiments and simulations
- Invented “postprocessing” estimator for free energies from irreversible computer simulations
- Developed estimator for equilibrium ensemble averages from nonequilibrium processes
- Derived analytical results showing the validity of new theorems in nonequilibrium statistical mechanics for a number of model systems

Graduate Student 8/2004-6/2007  
University of California, San Diego  
Advisor: J. Andrew McCammon

- Designed and conducted simulations to study crowding effects on HIV protease dynamics
- Analyzed simulations of neuraminidase from avian influenza and a acetylcholinesterase-fasciculin 2 complex
- Developed accelerated methods to estimate entropy
- Developed new methods for analyzing single-molecule pulling experiments

Undergraduate Student Intern 1/2004-7/2004  
Argonne National Laboratory, Argonne IL  
Advisor: Lee Makowski

- Observed macromolecular crowding effect on hemoglobin scattering patterns
- Developed software to analyze wide-angle X-ray scattering experiments

## Teaching Experience

Teaching Assistant 2005-2006  
University of California, San Diego

### Courses:

Chemistry 100A	Analytical Chemistry Laboratory	Winter 2006
Chemistry 126	Physical Chemistry – Quantum Mechanics and Spectroscopy	Fall 2005
Chemistry 115/215	Modeling Biological Macromolecules	Spring 2005
Chemistry 127	Physical Chemistry – Thermodynamics and Kinetics	Winter 2005

- Ran weekly discussion sections for approximately twenty students, held office hours, led reviews, and graded homework and exams (Chem 126 and 127)
- Supervised about twenty students during laboratory hours and graded reports (Chem 100A)
- Assisted students with computer modeling problems (Chem 115/215)

## Awards

Director's Postdoctoral Fellowship	8/2009-9/2011
Postdoctoral Intramural Research Training Award	8/2007-7/2009
NIH Molecular Biophysics Training Grant	8/2005-6/2007
Aguoron Kamen and Kaplan Fellowship	8/2004-8/2005
UC Berkeley Chancellor's Scholarship	8/2000-12/2003
National Merit Scholarship	8/2000-12/2003

## Service

Manuscript review for Biophysical Journal, Biopolymers, Journal of Chemical Physics, Journal of Molecular Biology, Journal of Physical Chemistry B, Journal of Structural Biology, and Physical Biology	
Universities Allied for Essential Medicines	
National Coordinating Committee	2006-2007
UC San Diego Chapter Coordinator	2005-2007
Speaker host for the UCSD Molecular Biophysics Training Grant	2007
Wrote popular science articles (10 articles) for the <i>Daily Californian</i> student newspaper at UC Berkeley	2002-2003

## Forthcoming Publications (in preparation/submitted)

1. **Minh DDL**, Makowski L. *Wide-angle X-ray solution scattering for protein-ligand binding: Multivariate curve resolution with Bayesian confidence intervals.*
2. **Minh DDL** et al., *The influence of ligand binding on adenylate kinase structural ensembles, as studied by wide-angle X-ray solution scattering and molecular dynamics simulation.*
3. Minh DL, **Minh DDL**. *Understanding and Generalizing the Hastings Algorithm.*

## Peer-Reviewed Publications

For links to articles, see electronic CV at <http://mccammon.ucsd.edu/~dminh/>

For up-to-date citation metrics, see <http://www.researcherid.com/rid/A-4655-2009>

1. Nilmeier JP, Crooks GE, **Minh DDL**, Chodera JD. *Nonequilibrium candidate Monte Carlo: A new tool for efficient equilibrium simulation*, Proceedings of the National Academy of Sciences USA, accepted. <http://arxiv.org/abs/1105.2278>
2. Minh DL, **Minh DDL**, Nguyen L. *Regenerative Markov Chain Monte Carlo for Any Distribution*, Communications in Statistics, accepted.
3. Makowski L, Gore D, Mandava S, **Minh DDL**, Park S, Rodi, DJ, and Fischetti RF. *X-ray solution scattering studies of the structural diversity intrinsic to protein ensembles*. Biopolymers, 95: 531-542 (August 2011). doi:[10.1002/bip.21631](https://doi.org/10.1002/bip.21631)

4. **Minh DDL**, Vaikuntanathan S. *Density-Dependent Analysis of Nonequilibrium Paths Improves Free Energy Estimates II. A Feynman-Kac Formalism*. Journal of Chemical Physics, 134(3): 034117 (January 2011). doi:[10.1063/1.3541152](https://doi.org/10.1063/1.3541152)
5. **Minh DDL**, Chodera JD. *Estimating equilibrium ensemble averages using multiple time slices from driven nonequilibrium processes: theory and application to free energies, moments, and thermodynamic length in single-molecule pulling experiments*. Journal of Chemical Physics, 134(2): 024111 (January 2011). doi:[10.1063/1.3516517](https://doi.org/10.1063/1.3516517)
6. **Minh DDL**. *Optimized replica gas estimation of absolute integrals and partition functions*. Physical Review E, 82(3): 031132 (September 2010). doi:[10.1103/PhysRevE.82.031132](https://doi.org/10.1103/PhysRevE.82.031132)
7. Qin S, **Minh DDL**, McCammon JA, Zhou, HX. *Method to Predict Crowding Effects by Postprocessing Molecular Dynamics Trajectories: Application to the Flap Dynamics of HIV-1 Protease*. Journal of Physical Chemistry Letters, 1(1):107–110 (January 2010). doi:[10.1021/jz900023w](https://doi.org/10.1021/jz900023w)
8. **Minh DDL**, Chodera JD. *Optimal estimators and asymptotic variances for nonequilibrium path-ensemble averages*. Journal of Chemical Physics, 131(13): 134110 (October 2009). doi:[10.1063/1.3242285](https://doi.org/10.1063/1.3242285)
9. **Minh DDL**. *Density-Dependent Analysis of Nonequilibrium Paths Improves Free Energy Estimates*. Journal of Chemical Physics, 130(20): 204102 (May 2009). doi:[10.1063/1.3139189](https://doi.org/10.1063/1.3139189)
10. **Minh DDL**, Adib AB. *Path integral analysis of Jarzynski's equality: Analytical results*. Physical Review E, 79(2): 021122 (February 2009). doi: [10.1103/PhysRevE.79.021122](https://doi.org/10.1103/PhysRevE.79.021122)
11. **Minh DDL**, McCammon JA. *Springs and Speeds in Free Energy Reconstruction from Nonequilibrium Single-Molecule Pulling Experiments*. Journal of Physical Chemistry B, 112(19): 5892-5897 (May 2008). doi:[10.1021/jp0733163](https://doi.org/10.1021/jp0733163)
12. **Minh DDL**, Adib AB. *Optimized free energies from bidirectional single-molecule force spectroscopy*. Physical Review Letters, 100(18): 180602 (May 2008). doi:[10.1103/PhysRevLett.100.180602](https://doi.org/10.1103/PhysRevLett.100.180602)
13. Makowski L, Rodi DJ, Mandava S, **Minh DDL**, Gore DB, Fischetti RF. *Molecular Crowding Inhibits Intramolecular Breathing Motions in Proteins*. Journal of Molecular Biology, 375(2): 529-546 (January 2008). doi:[10.1016/j.jmb.2007.07.075](https://doi.org/10.1016/j.jmb.2007.07.075)
14. **Minh DDL**, Hamelberg D, McCammon JA. *Accelerated Entropy Estimates with Accelerated Dynamics*. Journal of Chemical Physics, 127(15):154105 (October 2007). doi:[10.1063/1.2794754](https://doi.org/10.1063/1.2794754)
15. Amaro R, **Minh DDL**, Cheng L, Lindstrom WM, Olson AJ, Lin JH, Olson AJ, McCammon JA. *Remarkable Loop Flexibility in Avian Influenza N1 and its Implications for Antiviral Drug Design*. Journal of the American Chemical Society, 129(25):7764-7765 (June 2007). doi:[10.1021/ja0723535](https://doi.org/10.1021/ja0723535)
16. **Minh DDL**. *Multidimensional Potentials of Mean Force from Biased Experiments Along a Single Coordinate*. Journal of Physical Chemistry B, 111(16): 4137-4140 (April 2007). doi:[10.1021/jp068656n](https://doi.org/10.1021/jp068656n)
17. **Minh DDL**. *Free Energy Reconstruction from Experiments Performed Under Different Biasing Programs*. Physical Review E, 74(6): 061120 (December 2006). doi:[10.1103/PhysRevE.74.061120](https://doi.org/10.1103/PhysRevE.74.061120)

18. **Minh DDL**, Chang CE, Trylska J, Tozzini V, and McCammon JA. *The influence of macromolecular crowding on HIV-1 protease internal dynamics*. Journal of the American Chemical Society, 128(18): 6006-6007 (April 2006). doi:[10.1021/ja060483s](https://doi.org/10.1021/ja060483s)
19. **Minh DDL**, Bui JM, Chang CE, Jain T, Swanson JM, McCammon JA. *The entropic cost of protein-protein association: a case study on acetylcholinesterase binding to fasciculin-2*. Biophysical Journal, 89(4):L25-7 (October 2005). doi:[10.1529/biophysj.105.069336](https://doi.org/10.1529/biophysj.105.069336)