

# Brian Novak

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## Summary & Research Interests

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I have applied molecular simulations to various systems including biomolecular systems, interaction of biomolecules with non-biological materials, rapid solidification of metals and alloys, growth of Cu on TiN, and bubble nucleation. My main research interests are:

- Molecular and multiscale simulations of biomolecular systems
- Interaction of biomolecules with non-biological materials
- Interfacial phenomena and phase change

## Education

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### University of Notre Dame

PH.D., CHEMICAL ENGINEERING

2008/01

- **Molecular simulation studies of heterogeneous bubble nucleation: Effects of surface chemistry and topology**

### Kansas State University

B.S., CHEMICAL ENGINEERING

2002/05

### Additional Courses/Certifications

- Data Analyst with Python Track (2020/03)
- Python Programmer Track (2020/01)
- Medicinal Chemistry: The Molecular Basis of Drug Discovery (2019/11)
- Introduction to R (2019/10)
- Introduction to Time Series Analysis in Python (2019/10)
- Introduction to Programming with MATLAB (2015/12)

## Skills

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**Computer languages** Python, MATLAB, Tcl, Mathematica, Fortran, R

**MD related software** LAMMPS, GROMACS, NAMD, VMD, Ovito, Packmol

**Other** Linux, high performance computing

## Research Experience

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### Louisiana State University

*Molecular Simulation*

RESEARCH ASSOCIATE

2007/11 - present

- Function and dynamics of the enzyme biotin carboxylase
  - Showed that the ATP binding domain of biotin carboxylase (BC) is most stable in a closed configuration for a monomer and most stable in an open configuration for a dimer which may explain the loss of activity for monomers relative to dimers
  - Showed that there is communication between monomers of a BC dimer when ATP is bound in one monomer, and that the most stable state in this case is one with both monomers closed, supporting other evidence suggesting that a reaction occurs in only one monomer at a time
- Sequencing DNA using times-of-flight of single nucleotides as they pass through nanochannels
  - Performed initial simulations in nanoslits. Slit walls were composed of a single type of atom in a disordered arrangement approximating polymethyl methacrylate (PMMA). Smooth and rough walls were considered.
  - Assisted graduate students with running simulations with slit walls composed of PMMA and self-assembled monolayers.
  - Extrapolated simulation results to estimate the slit length required to obtain a given error rate as a metric to compare different surfaces.
- Bulk and interfacial properties of liquid metals & alloys
- Parameterization of phase field models for rapid solidification of Ti & Ti-Ni alloys using molecular dynamics simulations
  - Performed simulations to obtain kinetic coefficients for Ti. Assisted graduate student with setup and analysis of other kinetic coefficient and interfacial free energy simulations.
  - Wrote python code to analyze solid-liquid interfacial properties including velocity, interfacial free energy, and concentration profiles.
- Growth of Cu on TiN
  - Assisted graduate student with setup of simulations which showed that during deposition of Cu on TiN(100), bcc phase grows initially followed by martensitic transformation of bcc to twinned fcc(110)
- Self-assembly of bile salts or cationic linear peptide analogs (LPAs) and their interaction with lipid bilayers
  - Assisted graduate student and advisor with running bile salt simulations
  - Showed that LPAs with hydrocarbon connectors longer than 7 carbons form small, stable micelles at high concentrations.
  - Showed that longer LPA hydrocarbon connectors lead to deeper penetration into lipid bilayers.
  - Observed the existence of a long-lived trans-bilayer configuration for LPAs with 11 carbon hydrocarbon connectors.
- Behavior of alpha-tocopherol (vitamin E) in lipid bilayers
  - Performed initial simulations. Assisted graduate student with further simulations.
  - Analyzed trajectory data to show that the higher flip-flop rate of tocopherol at higher concentrations in thinner bilayers such as DMPC is associated with tocopherol clusters that span the bilayer.
- Interaction of lignin oligomers with lipid bilayers or  $\beta$ -cyclodextrin or microwaves
  - Assisted graduate student with the design and analysis of the simulations.
  - Suggested a normalized deuterium order parameter averaged over several carbon atoms in the lipid tails for monitoring the lipid gel-liquid crystalline phase transition.
- Interaction of poly(lactic-co-glycolic acid) (PLGA) nanoparticles with lipid bilayers
- Effect of DMSO on lipid bilayers
- Self-assembly of VECAR (vitamin E-carnosine) bolaamphiphiles
  - Assisted collaborators at Southeastern Louisiana University with simulation setup and analysis.
- Hybrid continuum/molecular dynamics simulations
  - Assisted graduate student with setup and analysis of simulations.
- Melting point estimation using unsupervised machine learning
  - Assisted collaborators in Physics Department with setup and analysis of simulations.

### University of Notre Dame

*Chemical Engineering*

GRADUATE RESEARCH ASSISTANT

2002/08 - 2007/09

- Showed that 4.5 nm indentations cause a large increase in nucleation rate relative to a smooth surface, but 1.5 nm indentations have little effect
- Applied a thermodynamic model using Mathematica that explained the location of critical bubble nuclei near flat surfaces and extended this model to geometric surface defects

### Kansas State University

*Chemistry*

UNDERGRADUATE RESEARCH ASSISTANT

1999/01 - 2001/01

- Showed the effects of solute-gel interactions by measuring electrochemiluminescence intensities of  $\text{Ru}(\text{bpy})_3^{2+}$  and diffusion coefficients of  $\text{Co}(\text{bpy})_3^{2+}$  in silica gels and organically modified silica gels

## Publications

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- Kavousi, S.; Novak, B.; Tong, X.; Moldovan, D. **Molecular Dynamics Simulation Study of the Positioning and Dynamics of  $\alpha$ -Tocopherol in Phospholipid Bilayers.** *Eur. Biophys. J.* 2021, Submitted.
- Tong, X.; Novak, B.; Kavousi, S.; Moldovan, D. **Single Nucleotides Moving Through Nanoslits Composed of Self-Assembled Monolayers via Equilibrium and Nonequilibrium Molecular Dynamics.** *J. Phys. Chem. B* 2021, 125 (4), 1259–1270.
- Kavousi, S.; Novak, B. R.; Hoyt, J.; Moldovan, D. **Interface Kinetics of Rapid Solidification of Binary Alloys by Atomistic Simulations: Application to Ti-Ni Alloys.** *Comput. Mater. Sci.* 2020, 184, 109854.
- Tong, X.; Moradipour, M.; Novak, B.; Kamali, P.; Asare, S. O.; Knutson, B. L.; Rankin, S. E.; Lynn, B. C.; Moldovan, D. **Experimental and Molecular Dynamics Simulation Study of the Effects of Lignin Dimers on the Gel-to-Fluid Phase Transition in DPPC Bilayers.** *J. Phys. Chem. B* 2019, 123 (39), 8247–8260.
- Kavousi, S.; Novak, B. R.; Baskes, M. I.; Zaeem, M. A.; Moldovan, D. **Modified Embedded-Atom Method Potential for High-Temperature Crystal-Melt Properties of Ti-Ni Alloys and Its Application to Phase Field Simulation of Solidification.** *Modelling Simul. Mater. Sci. Eng.* 2019, 28 (1), 015006.
- Muley, P. D.; Mobley, J. K.; Tong, X.; Novak, B.; Stevens, J.; Moldovan, D.; Shi, J.; Boldor, D. **Rapid Microwave-Assisted Biomass Delignification and Lignin Depolymerization in Deep Eutectic Solvents.** *Energy Convers. Manag.* 2019, 196, 1080–1088.
- Kavousi, S.; Novak, B. R.; Zaeem, M. A.; Moldovan, D. **Combined Molecular Dynamics and Phase Field Simulation Investigations of Crystal-Melt Interfacial Properties and Dendritic Solidification of Highly Undercooled Titanium.** *Comput. Mater. Sci.* 2019, 163, 218–229.
- Walker, N.; Tam, K.-M.; Novak, B.; Jarrell, M. **Identifying Structural Changes with Unsupervised Machine Learning Methods.** *Phys. Rev. E* 2018, 98 (5), 053305.
- Kim, H.-Y.; Novak, B. R.; Shrestha, B.; Lee, S. E.; Moldovan, D. **The Role of the Asymmetric Bolaamphiphilic Character of VECAR on the Kinetic and Structural Aspects of Its Self-Assembly: A Molecular Dynamics Simulation Study.** *Colloids Surf. Physicochem. Eng. Asp.* 2017, 523, 9–18.
- Xia, K.; Novak, B. R.; Weerakoon-Ratnayake, K. M.; Soper, S. A.; Nikitopoulos, D. E.; Moldovan, D. **Electrophoretic Transport of Single DNA Nucleotides Through Nanoslits: A Molecular Dynamics Simulation Study.** *J. Phys. Chem. B* 2015, 119 (35), 11443–11458.
- Sabliov, C. M.; Moldovan, D.; Novak, B.; Borel, T.; Whaley, M. **Cellular Fate of Delivery Systems and Entrapped Bioactives.** In *Nanotechnology and Functional Foods: Effective Delivery of Bioactive Ingredients*; Sabliov, C. M., Chen, H., Yada, R., Eds.; Wiley-Blackwell, 2015; pp 35–51.
- Novak, B. R.; Moldovan, D.; Nikitopoulos, D. E.; Soper, S. A. **Distinguishing Single DNA Nucleotides Based on Their Times of Flight through Nanoslits: A Molecular Dynamics Simulation Study.** *J. Phys. Chem. B* 2013, 117 (12), 3271–3279.
- Lin, J.; Novak, B.; Moldovan, D. **Molecular Dynamics Simulation Study of the Effect of DMSO on Structural and Permeation Properties of DMPC Lipid Bilayers.** *J. Phys. Chem. B* 2012, 116, 1299–1308.
- Novak, B. R.; Moldovan, D.; Waldrop, G. L.; de Queiroz, M. S. **Behavior of the ATP Grasp Domain of Biotin Carboxylase Monomers and Dimers Studied Using Molecular Dynamics Simulations.** *Proteins: Struct. Funct. Bioinform.* 2011, 79, 622–632.
- Novak, B. R.; Moldovan, D.; Waldrop, G. L.; de Queiroz, M. S. **Umbrella Sampling Simulations of Biotin Carboxylase: Is a Structure with an Open ATP Grasp Domain Stable in Solution?** *J. Phys. Chem. B* 2009, 113 (30), 10097–10103.
- Novak, B. R.; Maginn, E. J.; McCready, M. J. **An Atomistic Simulation Study of the Role of Asperities and Indentations on Heterogeneous Bubble Nucleation.** *J. Heat Trans.-T. ASME* 2008, 130.
- Novak, B. R.; Maginn, E. J.; McCready, M. J. **Comparison of Heterogeneous and Homogeneous Bubble Nucleation Using Molecular Simulations.** *Phys. Rev. B* 2007, 75.
- Collinson, M. M.; Novak, B. **Diffusion and Reactivity of Ruthenium (II) Tris(Bipyridine) and Cobalt (II) Tris(Bipyridine) in Organically Modified Silicates.** *J. Sol-Gel Sci. Technol.* 2002, 23, 215–220.
- Collinson, M. M.; Novak, B.; Martin, S. A.; Taussig, J. S. **Electrochemiluminescence of Ruthenium(II) Tris(Bipyridine) Encapsulated in Sol-Gel Glasses.** *Anal. Chem.* 2000, 72 (13), 2914–2918.

## Presentations

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### Oral - Invited

- **Molecular Dynamics Simulations of Biological Systems: Enzyme Conformational Change and Small Molecule (DNA) Sequencing**, Southeastern LA Univ. Chemistry & Physics Seminar (2010). In *Southeastern LA Univ. Chemistry & Physics Seminar*; 2010.

### Oral - Conference

- Tong, X.; Novak, B.; Moldovan, D. **Molecular Simulation of Single Nucleotides Moving through Nanoslits Composed of Self-Assembled Monolayers Terminated with Various Chemical Groups**. In *ACS Spring National Meeting*; 2018.
- Novak, B.; Raush, J.; Zhang, X.; Moldovan, D.; Meng, W.; Guo, S. **Properties of Liquid Ti Alloys from Electrostatic Levitation Experiments and Simulation**. In *APS March Meeting*; 2017.
- Novak, B.; Moldovan, D. **Self-Assembly of Linear Peptide Analogs and Their Interaction with Lipid Bilayers Using MD Simulations**. In *89th ACS Colloid & Surface Science Symposium*; 2015.
- Novak, B. R.; Lin, J.; Moldovan, D. **MD Simulations of Cationic Linear Peptide Analogs: Self-Assembly and Interaction with DPPC and DPPC/DPPS Lipid Bilayers**. In *ACS Fall National Meeting*; 2014.
- Novak, B. R.; Lin, J.; Moldovan, D. **Interaction of Cationic Linear Peptide Analogs with Negatively Charged Lipid Bilayers Studied with Molecular Dynamics Simulations**. In *ACS Spring National Meeting*; 2013.
- Novak, B.; Astete, C.; Sabliov, C.; Moldovan, D. **Interaction of PLGA nanoparticles with a DMPC bilayer studied using molecular dynamics simulations**. In *APS March Meeting*; 2012.
- Novak, B.; Xia, K.; Moldovan, D.; Nikitopoulos, D.; Soper, S. **Simulations of Single DNA Nucleotide Transport Through Nanoslits**. In *APS March Meeting*; 2011.
- Novak, B.; Moldovan, D.; Waldrop, G. L.; de Queiroz, M. S. **Opening/Closing Dynamics and Subunit Communication in Biotin Carboxylase**. In *Southwest & Southeastern Regional Meeting of the ACS*; 2010.
- Novak, B.; Moldovan, D.; Nikitopoulos, D.; Soper, S. **Molecular Dynamics Simulations of the Transport of Single DNA Nucleotides Through Nanochannels**. In *APS March Meeting*; 2010.
- Novak, B.; Maginn, E. J.; McCready, M. J. **Applying a Thermodynamic Model to Predict the Size of Surface Indentations That Affect Bubble Nucleation**. In *AIChE Annual Meeting*; 2007.
- Novak, B.; Maginn, E. J.; McCready, M. J. **Molecular Dynamics Investigation of Bubble Nucleation at a Solid Surface**. In *Midwest Thermodynamics and Statistical Mechanics Conference*; 2006.
- Novak, B.; Maginn, E. J.; McCready, M. J. **Effects of Geometric Defects on Superheated Heterogeneous Bubble Nucleation: A Molecular Dynamics Study**. In *AIChE Annual Meeting*; 2006.
- Novak, B.; Maginn, E. J.; McCready, M. J. **Superheated Homogeneous and Heterogeneous Bubble Nucleation Rates Using NPT and NP<sub>zz</sub>T Molecular Dynamics: Effects of Surface Interactions**. In *AIChE Annual Meeting*; 2005.

### Poster - Conference

- Novak, B.; Moldovan, D.; Waldrop, G.; de Queiroz, M. **Insights into the Opening and Closing Dynamics of Biotin Carboxylase**. In *APS March Meeting*; 2010.
- Novak, B.; Moldovan, D.; Waldrop, G.; de Queiroz, M. **Opening and Closing of Biotin Carboxylase: Free Energies and Mean First Passage Times**. In *Mardi Gras Conference*; 2010.
- Novak, B.; Moldovan, D.; Nikitopoulos, D.; Soper, S. **Molecular Dynamics Simulations for Calculation of Times of Flight of Single DNA Nucleotides Driven through Nanochannels**. In *Mardi Gras Conference*; 2010.
- Novak, B.; Lin, J.; Moldovan, D.; Jha, S.; Soper, S.; Nikitopoulos, D. **MD Simulations of DNA Mononucleotide Transport through Nanochannels**. In *21st EPSCoR National Conference*; 2009.
- Novak, B.; Moldovan, D.; Waldrop, G.; de Queiroz, M. **Umbrella Sampling Simulations of the Closure of Biotin Carboxylase**. In *International Conference on Multiscale Materials Modeling*; 2008.

**Author only**

- Tong, X.; Maradipour, M.; Novak, B.; Knutson, B.; Rankin, S.; Lynn, B.; Moldovan, D. **Molecular Dynamics Simulation Study of the Effect of Lignin Dimers on the Gel to Liquid-Crystalline Transition Temperature in DPPC Bilayers.** In *ACS Spring National Meeting*; 2019.
- Kavousi, S.; Novak, B.; Moldovan, D. **Phase Field Modeling of Rapid Solidification of Ti-Ni Alloy Parameterized Using Interfacial Properties Calculated from Atomistic Simulations.** In *MRS Fall Meeting*; 2019.
- Kavousi, S.; Novak, B.; Moldovan, D. **Combined Molecular Dynamics and Phase Field Simulation Study of Directional Solidification of NiTi Alloy.** In *TMS Annual Meeting & Exhibition*; 2019.
- Kavousi, S.; Novak, B.; Moldovan, D. **Molecular Dynamics Simulation Study of Alpha-Tocopherol Interaction with Lipid Bilayers.** In *ACS Spring National Meeting*; 2018.
- Walker, N.; Novak, B.; Tam, K. M.; Moldovan, D.; Jarrell, M. **Ab Initio Calculations of Transport in Titanium and Aluminum Mixtures.** In *APS March Meeting*; 2017.
- Tam, K. M.; Novak, B.; Walker, N.; Moldovan, D.; Jarrell, M. **Finite Size Scaling of the First Order Transition of Molecular Systems.** In *APS March Meeting*; 2017.
- Raush, J.; Novak, B.; Zhang, X.; Moldovan, D.; Meng, W.; Guo, S. **Measurement and Calculation of Liquid Ti Alloy Properties with Application to 3D Printing.** In *4th World Congress on Integrated Computational Materials Engineering*; 2017.
- Shrestha, B.; Kim, H.-Y.; Lee, S.; Novak, B.; Moldovan, D. **Self-Assemblies of Novel Molecules, VECAR.** In *APS March Meeting*; 2015.
- Novak, B.; Lin, J.; Moldovan, D. **Investigation of Linear Peptide Analogs Self-Assembly and Interaction with DPPC and DPPC/DPPS Lipid Bilayers: A Molecular Dynamics Simulation Study.** In *The Central and Eastern European Conference on Health and the Environment*; 2014.
- Xia, K.; Lin, J.; Nikitopoulos, D.; Moldovan, D. **Molecular Dynamics Simulation of Electrically Driven Single DNA Nucleotides through Nanoslits.** In *ACS Spring National Meeting*; 2013.
- Lin, J.; Novak, B.; Moldovan, D. **Molecular Dynamics Simulation Study of Bile Salt Aggregation and Interaction with Vitamin E.** In *ACS Spring National Meeting*; 2013.
- Xia, K.; Novak, B.; Moldovan, D.; Nikitopoulos, D.; Soper, S. **MD Simulation Study of the Effect of Electric Field on the Dynamics of DNA Nucleotides in Hydrophobic Nanoslits.** In *ACS Spring National Meeting*; 2012.
- Novak, B.; Xia, K.; Nikitopoulos, D.; Soper, S.; Moldovan, D. **Atomistic Simulation Study of Single DNA Nucleotide Transport through Nanoslits.** In *ACS Spring National Meeting*; 2012.
- Novak, B.; Lin, J.; Moldovan, D. **Molecular Dynamics Simulation of Adsorption and Positioning of Vitamin E in DMPC Lipid Bilayers: Implication for Their Antioxidant Inhibition.** In *Colloids and Nanomedicine*; 2012.
- Lin, J.; Novak, B.; Moldovan, D. **Molecular Dynamics Simulation of Bile Salts Micelle Self-Assembly in Aqueous Solutions.** In *ACS Spring National Meeting*; 2012.
- Moldovan, D.; Alapati, R.; Novak, B.; Devireddy, R. **Molecular Dynamics Simulation Study of Structural Changes and Pore Formation in Phospholipid Bilayers in the Presence of Dimethylsulfoxide.** In *APS March Meeting*; 2010.
- Novak, B.; Xia, K.; Moldovan, D.; Nikitopoulos, D.; Soper, S. **Molecular Dynamics Simulations of the Movement of Single DNA Nucleotides through Nanoslits.** In *Southwest & Southeastern Regional Meeting of the ACS*; 2010.
- Lao, J.; Lin, J.; Xia, K.; Sabliov, C.; Moldovan, D. **Molecular Dynamics Simulation of Self-Assembly of Span80 into Micelles and Their Interaction with Vitamin E.** In *Mardi Gras Conference*; 2010.
- Chantiwas, R.; Hupert, M.; Lopez, J.; Datta, P.; Gottert, J.; Novak, B.; Moldovan, D.; Jha, S.; Park, S.; Murphy, M.; et al. **Transport of Single Molecules through Nanochannels: A Novel Approach to DNA Sequencing.** In *International Conference on Miniaturized Systems for Chemistry and Life Sciences*; 2009.

**Peer Reviewing**

- Improved kinetic description of fast relaxation of cylindrical micelles, *Physica A*, 2018-10-11
- Shuffled lipidation pattern and degree of lipidation determines the membrane interaction behavior of a linear cationic membrane-active peptide, *Mol. Pharm.*, 2018-04-29
- Rapid Transport of Deformation-Tuned Nanoparticles across Biological Hydrogels and Cellular Barriers, *Nat. Commun.*, 2017-12-05

**Leadership & Teaching Experience****Louisiana State University**

Baton Rouge, LA

## MENTOR

2007/11 - present

- 7 graduate students
- 10 undergraduate students

## MATLAB COURSE INSTRUCTOR

2015/Fall

**University of Notre Dame**

Chemical Engineering

## TEACHING ASSISTANT

2002/08 - 2004/05

- Chemical Engineering Laboratory II (Fall 2002) – Supervised 3 experiments
- Chemical Engineering Laboratory I (Spring 2003) – Supervised 2 experiments
- Introduction to Chemical Engineering (Fall 2003) – Graded homework and tests
- Global Climate Change (Spring 2004) – Homework solutions and grading