Brian Novak

(620) 214-1850 | brian.novak.simulation@gmail.com | bnovak1 | briannovak

Summary & Research Interests

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

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

Computer languages	Python, MATLAB, Tcl, Mathematica, Fortran, R
MD related software	LAMMPS, GROMACS, NAMD, VMD, Ovito, Packmol
Other	Linux, high performance computing

Research Experience

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.
- 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.
- 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 bulk and cluster simulations to show that Cu(100) grows on TiN(100) while Cu(110) grows on TiN(310)
  - Applied minima hopping global optimization to study initial Cu cluster growth
- 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 β-cyclodextrin or microwaves
  - Assisted graduate student with the design 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
- 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 $Ru(bpy)_3^{2+}$ and diffusion coefficients of $Co(bpy)_3^{2+}$ in silica gels and organically modified silica gels

Publications

- 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* 2020, Submitted.
- Kavousi, S.; Novak, B.; Tong, X.; Moldovan, D. **Molecular Dynamics Simulation Study of the Positioning and Dynamics of α-Tocopherol in Phospholipid Bilayers**. *Eur. Biophys. J.* 2020, Submitted.
- 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

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 $NP_{zz}T$ 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

Louisiana State University

Baton Rouge, LA

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