CHANG WOON JANG, Ph.D

Materials and Data Scientist

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EDUCATION

University of Pennsylvania, *Philadelphia, PA*
Data Science and Visualization Boot Camp

Mississippi State University, *Mississippi State, MS*
Ph.D., Aerospace Engineering

Pukyong National University, *Busan, South-Korea*
Bachelor of Science, Physics

WORK EXPERIENCES

Materials Scientist, *KBR Wyle, Mountain View, CA* Dec. 2018-Current
NASA Ames Research Center
Development of computational analysis codes for simulating aerospace grade composite materials. Development of QSAR from protein-drug docking simulations. Publish research papers.

Research Scientist, *Department of Materials Chemistry* June. 2017-May. 2018
Nagoya University
Development of computational analysis codes, which enable predicting properties of perfluorosulfonic acid polymeric battery membrane at the atomistic and coarse-graining simulations. Publish research papers.

Postdoctoral Research Associate, *Biological and Chemical Engineering* Sep. 2012-May. 2017
Drexel University
Performed research using atomistic simulations to characterize properties polymers, understand mechanisms of their atomistic behaviors, and build structural-property relationships. Publish research papers.

COMPUTER SKILLS

Simulation Packages
LAMMPS, Materials Studio, GROMACS, COMSOL, ABAQUS

Machine Learning Python Libraries
Scikit-learn, Numpy, Scipy, Pandas, Matplotlib

Software/Applications
Autodock, Schrodinger Software, MOE, VOTCA, Jmol, Packmol, ChemSketch, VMD, Xmgrace, GNU Plot, Avogardro, Ambertools, MS Office

Languages and Scripts
C/C++, Python, Perl, AWK, SED, TCL, Linux Shell Script

LIST OF PUBLICATIONS

Book Chapter (HYPERLINK)

Lacy, T., Gwaltney, S. R., Pittman, C., Toghiani, H., **Jang, C**., Nouranian, S., and Yu, J. (May 2011). "Some Key Issues in Multi-Scale Modeling of Thermoset Nanocomposites/Composites" In S. M. Arnold, T. Wong (Eds.), Tools, Models, Databases, and Simulation Tools Developed and Needed to Realize the Vision of Integrated Computational Materials Engineering, Materials Park, OH: ASM International.

Peer-Reviewed Journal Articles (HYPERLINK)

1. **Jang, C**., Kang, J. H., Palmieri, F. L., Hudson, T. B., Brandenburg, C. J., Lawson, J. W. "Molecular Dynamics Investigation of the Structural and Mechanical Properties of Off-Stoichiometric Epoxy Resins" *ACS Applied Polymer Materials* 2021, 3, 2950.
2. Kuo, A-T., Miyazaki, Y., **Jang, C**., Nielsen, S. O., Okazaki, S., Shinoda, W. "Large-scale Molecular Dynamics Simulation of Perfluorosulfonic Acid Membranes: Remapping Coarse-grained to All-atomistic Simulations" *Polymer* 2019, 181, 121766.
3. Payal, R. S., Fujimoto, K., **Jang, C**., Wataru, Shinoda., Takei, Y., Shima, H., Tsunoda, K., Okazaki, S. "Molecular Mechanism of Material Deformation and Failure in Butadiene Rubber: Insight from All-atom Molecular Dynamics Simulation using a Bond Breaking Potential Model" *Polymer*, 2019, 170, 113-119.
4. Yang, JH., Srikanth, A., **Jang, C**., Abrams, C. F. "Relationships between molecular structure and thermomechanical properties of bio-based thermosetting polymers" *Journal of Polymer Science Part B: Polymer Physics*. 2017, 55, 285-292.
5. **Jang, C**., Abrams, C. F. "Thermal and Mechanical Properties of Thermosetting Polymers using Coarse-grained Simulation" *The European Physical Journal Special Topics*. 2016, 225, 1775-1783.
6. **Jang, C**., Sharifi, M., Palmese, G. R., Abrams, C. F. "Toughness Enhancement of Thermosetting Polymers Using a Novel Partially Reacted Substructure Curing Protocol: A Combined Molecular Simulation and Experimental Study" *Polymer*. 2016, 90, 249-255.
7. Sharifi, M., **Jang, C**., Abrams, C. F., Palmese, G. R. "Epoxy Polymer Network with Improved Thermal and Mechanical Properties via Controlled Dispersion of Reactive Toughening Agents" *Macromolecules*. 2015, 48(20), 7495-7502.
8. **Jang, C**., Sirk, T., Andzelm, J., Abrams, C. F. "Comparison of Crosslinking Algorithms in Molecular Dynamics simulations of Thermosetting Polymer" *Macromolecular Theory and Simulation*. 2015, 24(3), 260-270.
9. Sharifi, M., **Jang, C**., Abrams, C. F., Palmese, G. R. "Toughened Epoxy Polymers via Rearrangement of Network Topology" *Journal of Materials Chemistry A*. 2014, 2(38), 16071-16082.
10. **Jang, C**., Sharifi, M., Palmese, G. R., Abrams, C. F. "Crosslink Network Rearrangement via Reactive Encapsulation of Solvent in Epoxy Curing: A Combined Molecular Simulation and Experimental Study" *Polymer*, 2014, 55(16), 3282-3289.
11. **Jang, C**., Hutchins, J., Yu, J. "Carbon Nanofiber-reinforced Polymeric Nanocomposites" *Carbon Letters*, 2013, 14(4), 197-205.
12. **Jang, C**., Lacy, T., Gwaltney, S. R., Toghiani, H., and Pittman, C. "Interfacial Shear Strength of Cured Vinyl Ester Resin-Graphite Nanoplatelet from Molecular Dynamics Simulations" *Polymer*, 2013, 54(13), 3282-3289.
13. **Jang, C**., Lacy, T., Gwaltney, S. R., Toghiani, H., and Pittman, C. "Relative Reactivity Volume Criterion for Cross-Linking: Application to Vinyl Ester Resin Molecular Dynamics Simulations" *Macromolecules*, 2012, 45(11), 4876-4885.

14. **Jang, C**., Nouranian, S., Lacy, T., Gwaltney, S. R., Toghiani, H., and Pittman, C. Jr. "Molecular Dynamics Simulation of Oxidized Vapor-Grown Carbon Nanofiber Surface Interactions with Vinyl Ester Resin Monomers" *Carbon*, 2012, 50(3), 748-760.
15. Nouranian, S., **Jang, C**., Lacy, T., Gwaltney, S. R., Toghiani, H., and Pittman, C. Jr. "Molecular Dynamics Simulations of Vinyl Ester Resin Monomer Interactions with a Pristine Vapor-Grown Carbon Nanofiber and Their Implications for Composite Interphase Formation" *Carbon*, 2011, 49(10), 3219-3232.

Conference Proceedings

1. **Jang, C**., Majid Sharifi., Giuseppe R. Palmese., Cameron F. Abrams (Sep 2015). Partially Reacted Substructures Method for Thermoset Epoxies Studied Using Molecular Dynamics Simulations, 2015 ASC 30 Technical Conference, September 28-30, Michigan State University, MI.
2. **Jang, C**., Majid Sharifi., Giuseppe R. Palmese., Cameron F. Abrams " Molecular Dynamics Simulation Study of Reactive Encapsulation of Solvent in Epoxy Curing, 2014 ASC 29/US-Japan 16/ASTM D30 Conference, September 8-10, UC San Diego, CA.
3. **Jang, C**., Lacy, T., Gwaltney, S. R., Toghiani, H., and Pittman, C. Jr. "Molecular Dynamics Simulation of Vinyl Ester Resin Crosslinking." To appear in the Proceeding of 53 rd. AIAA/ASME/ASCE/ASC Structures, Structural Dynamics, and Materials Conference, April 2012, Honolulu, Hawaii.
4. **Jang, C**., Lacy, T., Gwaltney, S. R., Toghiani, H., and Pittman, C. Jr. "Interfacial Shear Strength of a Graphene/Vinyl Ester Composite Determined by Molecular Dynamics Simulations." to appear in the The American Society for Composites 27th Technical Conference, the 15th US-Japan Conference on Composite Materials and the ASTM-D30 Meeting, October, 1-3, Arlington, TX.

PRESENTATIONS

1. "Development of Atomistic Molecular Dynamics Simulation to Characterize Microscopic Fracture Behavior of Epoxy Resins", *AIChE*, San Francisco, CA, November **2020**. (Oral)
2. "Property Prediction of Offset Polymers", *APS Meeting*, Denver, CO, March **2020**. (Oral)
3. "Polymer Electrolyte Membrane", *IMPACT Meeting*, Zushi, Japan, October **2018**. (Poster)
4. "Epoxy Molecular Simulations", *MEDE Fall Meeting*, Towson, MD, October **2016**. (Poster)

4. "Epoxy Molecular Simulations", *Summer 2016 MEDE Composites CMRG Meeting*, August **2016**. (Oral)
5. "Molecular Dynamics Simulation Study of Thermosetting Polymers from Atomistic to Mesoscopic Scales", *MEDE Composites CMRG Conference Call*, May **2016**. (Oral)
6. "Coarse-Grained Molecular Dynamics Simulations of DGEBA/POP-DA Crosslinked Thermosets", *Mach Conference*, Annapolis, MD, April **2016**. (Poster)
7. "Partially Reacted Substructures Method for Thermoset Epoxies Studied Using Molecular Dynamics Simulations", *ASC 30 Technical Conference*, Michigan State University MI, September **2015**. (Oral)
8. "Understanding Properties Enhancement of Thermoset Epoxies Cured via Partially Reacted Substructures", *Mach Conference*, Annapolis, MD, April **2015**. (Oral)
9. "Molecular Dynamics Simulation Study of Reactive Encapsulation of Solvent in Epoxy Curing", *ASC 29/US-Japan 16/ASTM D30 Conference*, San Diego, CA, September **2014**. (Oral)
10. "Comparison of Crosslinking Algorithms on Material Properties and Network Structure of Simulated Epoxies", *MEDE Fall Meeting*, Towson, MD, October **2014**. (Poster)
11. "Characterizing Molecular-Scale Void Space in Epoxies using All-atom Molecular Simulations", *Mach Conference*, Annapolis, MD, 2014. (Oral)

12. “Molecular Dynamics Simulation of Vinyl Ester Resin Crosslinking.”, *53 rd. AIAA/ASME/ASCE/ASC Structures, Structural Dynamics, and Materials Conference*, Honolulu Hawaii, April **2012**. (Oral)
13. “Molecular Dynamics Simulations of An Oxidized Vapor-Grown Caron Nanofiber and Vinyl Ester Resin Interactions Leading to a Possible Interphase Formation in the Cured Nanocomposites.”, *AIChE Annual Meeting*, Salt lake City, UT, October **2011**. (Oral)