Jan-Michael Y. Carrillo

Center for Nanophase Materials Sciences
Oak Ridge National Laboratory – Oak Ridge, TN 37831

☏ (865) 576 4860   •   ✉ carrillojy@ornl.gov

Education

University of Connecticut   **Storrs, CT**
Ph.D. Polymer Science   *2009*

University of the Philippines   **Quezon City, Philippines**
M.S. Environmental Engineering   *2003*

University of the Philippines   **Quezon City, Philippines**
B.S. Chemical Engineering   *1998*
Honors: *cum laude*

Research Experience

Oak Ridge National Laboratory   **Oak Ridge, TN**
Research Staff   *2019–Present*
Center for Nanophase Materials Sciences

Oak Ridge National Laboratory/University of Tennessee Knoxville   **Oak Ridge, TN**
Research Scientist   *2015-2019*
Joint Institute for Computational Sciences

Oak Ridge National Laboratory   **Oak Ridge, TN**
Postdoctoral Fellow   *2012-2014*
National Center for Computational Sciences

University of Connecticut   **Storrs, CT**
Postdoctoral Fellow   *2010-2012*
Department of Physics

Honors and Awards

Oak Ridge Leadership Computing Facility
OLCF SummitPLUS Allocation Award   *2023*
"Modeling Key Cell Cycle Processes in Bacteria"

U.S. Department of Energy, Office Of Science
ASCR Leadership Computing Challenge (ALCC) Award   *2020*
"Nonlinear Rheology of Entangled Polymers"

Center for Nanophase Materials Sciences
Distinguished Scientific Paper   *2018*
"Molecular Dynamics Investigation of the Relaxation Mechanism
of Entangled Polymers after a Large Step Deformation"

Georgia Tech Energy Frontier Research Center
Best Paper Award   *2016*
"Unraveling the Dynamics of Aminopolymer/Silica Composites"

International Data Corporation (IDC)
High Performance Computing Innovation Excellence Award   *2013*
Large-scale Organic Photovoltaic Simulations

University of Connecticut
Doctoral Dissertation Fellowship   *2006*

Philippine Board of Chemical Engineering
Topnotcher (5th place) Professional Licensure Examination   *1998*

Philippine Department of Science and Technology
Science Education Institute - University Scholarship Award   *1993-1998*

Online Profiles and Metrics

https://scholar.google.com/citations?user=pgXvCjcAAAAJ&hl

http://orcid.org/0000-0001-8774-697X

Selected Invited Talks (2019–2023)

Tutorial: MD Simulations of Polymers   *2019–2021 (Summer)*
Cyber Training Summer School, Rensselaer Polytechnic Institute (RPI) Troy NY

From Lipid Vesicles to Lipid Onions: A Molecular Dynamics Simulation Study   *2019*
ACS Spring Meeting, Orlando FL

Assembly of Charged Star Block Copolymers at the Oil-Aqueous Interface   *2022*
ACS Fall Meeting, Chicago IL (Virtual)

Multiscale Molecular Dynamics Simulations of Soft Matter and Polymeric Systems   *2022*
Chemical Society of the Philippines, Manila, Philippines (Virtual)

Design of Charged Star Block Copolymer Surfactants via ML and CG MD Simulations   *2023*
ACS Fall Meeting, San Francisco CA

Beyond Implicit Solvents: Advancing Soft Matter Simulations with Explicit Solvent MD *2023*
VT-ORNL Soft Matter and Biological Physics Symposium, Blacksburg VA

Selected Contributed Talks (2019–2023)

The Effects of Mesogen Spacer and Linker on the Actuation of Liquid Crystal Elastomers　　*2019*
APS March Meeting, Boston MA

Molecular Dynamics Simulations of a Polymer Star under Shear Flow　　*2020*
APS March Meeting, Denver CO (APS was cancelled but presented at ORNL)

Diblock Copolymer Melts of Linear Chains, Rings and Trefoil Knots in Lamellar Morphology　　*2021*
APS March Meeting, Nashville TN (Virtual)

Assembly of Polyelectrolyte Star Block Copolymers at the Oil-Water Interface　　*2022*
APS March Meeting, Chicago IL (Virtual)

CG Explicit-Solvent MD Simulations of Polyelectrolyte Chains in Solution　　*2023*
APS March Meeting, Las Vega NV

Professional and Synergistic Activities

1. Service to the Discipline

   - Member and contributor to ACS and APS.
   - Contributes to AICHE and ACNS (American Conference on Neutron Scattering), including talks and posters through collaborators.
   - Session Chair for the 2011 APS March Meeting on "Biopolymers: Molecules, Solutions, Networks, and Gels" in Dallas, MA.
   - Session Chair for the 2012 APS March Meeting on "Elastomers and Gels" in Boston, MA.
   - Session Chair for the 2014 AICHE Meeting on "Thin Film Block Copolymer Self-Assembly and Morphology" in Atlanta, GA.

2. Community Outreach

   - Provided a basic tutorial on how to perform coarse-grained molecular dynamics simulations of polymers at the Cyber Training Summer School at Rensselaer Polytechnic Institute (RPI) during the summers of 2019-2021.
   - Maintained and provided codes and scripts to support the Cyber Training Summer School. (Link: `https://code.ornl.gov/jyw/cyber-training-summer-school`)
   - Provided efficient tools, utilizing GPUs, for analyzing coarse-grained molecular dynamics simulations trajectories from LAMMPS, available to the broad community. (Link: `https://code.ornl.gov/jyw/LAMMPS-DATA-ANALYSIS`)

3. Peer Review

- Peer reviewer for journals from the American Physical Society, American Chemical Society, Royal Society of Chemistry, Elsevier, Wiley, etc.

4. Grant Review

- NIST NCNR Proposal Beam Time allocation reviewer
- DOE INCITE computational readiness (CR) reviewer
- NSF Cyberinfrastructure for Sustained Scientific Innovation (CSSI) panel reviewer
- NSF Division of Materials Research (DMR) reviewer
- ACS PRF scientific evaluator

5. Mentoring

- ORNL Graduate Student Intern (Summer 2021 – Rishabh Guha)
- ORNL Next Generation STEM Internship Program (NGSI) (Summer 2023 - Adarsh Muralidharan)
- Close mentorship to postdocs and graduate students of collaborators (e.g., Wensheng Xu, Jihong Ma, Zhiqiang Shen, Yashavi Bajaj, Hyun June Moon, etc.)

6. Service to ORNL

- OLCF DD allocation computational feasibility reviewer
- LDRD reviewer
- Publication reviewer (RESolution)
- CNMS user project feasibility reviewer
- CNMS workshop chair and contributor
- NSD-CNMS workshop contributor

In the News and Highlights

- BES October 2023 Highlight "Modeling Polymers for Next-Generation Manufacturing and Sustainability"
https://www.energy.gov/science/bes/articles/modeling-polymers-next-generation-manufacturing-and-sustainability

- OLCF July 2023 Highlight "Advancing nanoscience through largescale MD simulations: The OLCF teams with ORNL's Center for Nanophase Materials Sciences and Stony Brook University to learn how cicada wings kill bacteria"
https://www.olcf.ornl.gov/2023/07/13/advancing-nanoscience-through-largescale-md-simulations/

- ORNL April 2022 Research Highlight "Machine Learning Enables Inversion of Neutron Scattering Data"

https://www.ornl.gov/research-highlight/machine-learning-enables-inversion-neutron-scattering-data

- ORNL PSD July 2021 Research Highlight "Ion Pairing Mediates Molecular Organization Across Liquid/Liquid Interfaces"
  https://www.ornl.gov/research-highlight/ion-pairing-mediates-molecular-organization-across-liquidliquid-interfaces

- ONRL December 2020 Research Highlight "Ionic Junctions Enable Delicate Control over Microphase Domain Features in Diblock Copolymers"
  https://www.ornl.gov/research-highlight/ionic-junctions-enable-delicate-control-over-microphase-domain-features-diblock

- PHYS.ORG September 2020 News "Nanomaterials— short polymers, big impact"
  https://phys.org/news/2020-09-nanomaterials-short-polymers-big-impact.html

- ORNL September 2020 Research Highlight "Controlling the Formation of Double Membrane Vesicles"
  https://www.ornl.gov/research-highlight/controlling-formation-double-membrane-vesicles

- OLCF August 2020 Highlight "ALCC Program Awards Nearly 6 Million Summit Node Hours Across 31 Projects"
  https://www.olcf.ornl.gov/2020/08/05/alcc-program-awards-nearly-6-million-summit-node-hours-across-31-projects/

- ORNL November 2019 Research Highlight "Polymer Architecture Enables Protein Resistant Surfaces"
  https://www.ornl.gov/research-highlight/polymer-architecture-enables-protein-resistant-surfaces

- OLCF April 2018 Highlight "A Problem with Polymer Theory: ORNL scientists use simulation to back up experimental challenge to popular theory"
  https://www.olcf.ornl.gov/2018/04/16/a-problem-with-polymer-theory/

- ORNL April 2017 Research Highlight "Tuning Polymer Molecule Architecture for Targeted Self-Organization"
  https://www.ornl.gov/news/tuning-polymer-molecule-architecture-targeted-self-organization

- ORNL March 2017 Research Highlight "Small nanoparticles have surprisingly big effects on polymer nanocomposites"
  https://www.ornl.gov/news/small-nanoparticles-have-surprisingly-big-effects-polymer-nanocomposites

- OLCF June 2014 Highlight "Titan Shines at American Physical Society March Meeting"
  https://www.olcf.ornl.gov/2014/06/30/titan-shines-at-american-physical-society-march-meeting/

- OLCF April 2014 Highlight "Simulation Solves Mystery of How Liquid-Crystal Thin Films Disintegrate"
  `https://www.olcf.ornl.gov/2014/04/11/simulation-solves-mystery-of-how-liquid-crystal-thin-films-disintegrate/`

- OLCF March 2013 Highlight "Seeing is Believing: New OLCF visualization lab showing early promise"
  `https://www.olcf.ornl.gov/2014/03/18/seeing-is-believing/`

- OLCF August 2013 Highlight "Titan Sheds Light on Unknowns in Organic Photovoltaic Research"
  `https://www.olcf.ornl.gov/2013/08/21/titan-sheds-light-on-unknowns-in-organic-photovoltaic-research/`

- OLCF July 2013 Highlight "Early Molecular Dynamics Research Blazes Through Titan's New GPUs"
  `https://www.olcf.ornl.gov/2013/07/25/early-molecular-dynamics-research-blazes-through-titans-new-gpus/`