Jan-Michael Y. Carrillo

Education

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

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

1998 **B.S. Chemical Engineering**, *University of the Philippines*, Quezon City, Philippines.

Research Interests

Focusing on the use of computational methods, such as Molecular Dynamics simulations, to elucidate the effects of soft matter microscopic parameters (*e.g.*, polymer chain persistence length) on experimentally measurable macroscopic properties (*e.g.,* material stress–strain curve). The simulations provide insights on the interpretation of experiments, such as those of neutron scattering (*e.g.,* SANS, NSE, NR). In addition, the simulations serve to inspire novel characterization experiments and influence the direction of new polymeric or colloidal material syntheses. Simulation results are reflected in more than 40 peer reviewed articles with cumulative citations > 500 (h-index $= 13$ (Web of Science), h-index $= 14$ (Google Scholar)).

Research Experience

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

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

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

2004-2009 **Graduate/Research Assistant**, *University of Connecticut*, Storrs, CT.
Institute of Materials Science

Honors and Awards

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

2006 **Doctoral Dissertation Fellowship**, *University of Connecticut.*

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

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

Publications

[1] Zhen Cao, Jan-Michael Y Carrillo, Sergei S Sheiko, and Andrey V Dobrynin. Computer simulations of bottle brushes: From melts to soft networks. *Macromolecules*, 48(14):5006–5015, 2015.

[2] Jan-Michael Y Carrillo, Shiwang Cheng, Rajeev Kumar, Monojoy Goswami, Alexei P Sokolov, and Bobby G Sumpter. Untangling the effects of chain rigidity on the structure and dynamics of strongly adsorbed polymer melts. *Macromolecules*, 48(12):4207–4219, 2015.

[3] W Michael Brown, Jan-Michael Y Carrillo, Nitin Gavhane, Foram M Thakkar, and Steven J Plimpton. Optimizing legacy molecular dynamics software with directive-based offload. *Computer Physics Communications*, 195:95–101, 2015.

[4] Zhen Cao, Mark J Stevens, Jan-Michael Y Carrillo, and Andrey V Dobrynin. Adhesion and wetting of soft nanoparticles on textured surfaces: Transition between wenzel and cassie–baxter states. *Langmuir*, 31(5):1693–1703, 2015.

[5] Rajeev Kumar, Jan-Michael Y Carrillo, Monojoy Goswami, and Bobby G. Sumpter. Insights obtained from modeling of organic photovoltaics: Morphology, interfaces, and coupling with charge transport. In *Organic Solar Cells: Materials, Devices, Interfaces, and Modeling*, pages 113–140. CRC Press, 2015.

[6] Che-Nan Sun, Thomas A Zawodzinski, Wyatt E Tenhaeff, Fei Ren, Jong Kahk Keum, Sheng Bi, Dawen Li, Suk-Kyun Ahn, Kunlun Hong, Adam J Rondinone, Jan-Michael Y Carrillo, Changwoo Do, Bobby G Sumpter, and Jihua Chen. Nanostructure enhanced ionic transport in fullerene reinforced solid polymer electrolytes. *Physical Chemistry Chemical Physics*, 17(12):8266–8275, 2015.

[7] Steven J Woltornist, Jan-Michael Y Carrillo, Thomas O Xu, Andrey V Dobrynin, and Douglas H Adamson. Polymer/pristine graphene based composites: From emulsions to strong, electrically conducting foams. *Macromolecules*, 48(3):687–693, 2015.

[8] Suk-kyun Ahn, Jan-Michael Y Carrillo, Youngkyu Han, Tae-Hwan Kim, David Uhrig, Deanna L Pickel, Kunlun Hong, S Michael Kilbey, Bobby G Sumpter, Gregory S Smith, and Changwoo Do. Structural evolution of polylactide molecular bottlebrushes: Kinetics study by size exclusion chromatography, small angle neutron scattering, and simulations. *ACS Macro Letters*, 3(9):862–866, 2014.

[9] Jan-Michael Y Carrillo and Andrey V Dobrynin. Salt effect on osmotic pressure of polyelectrolyte solutions: Simulation study. *Polymers*, 6(7):1897–1913, 2014.

[10] Jan-Michael Y Carrillo and Bobby G Sumpter. Structure and dynamics of confined flexible and unentangled polymer melts in highly adsorbing cylindrical pores. *The Journal of chemical physics*, 141(7):074904, 2014.

[11] Trung Dac Nguyen, Jan-Michael Y Carrillo, Michael A Matheson, and W Michael Brown. Rupture mechanism of liquid crystal thin films realized by large-scale molecular simulations. *Nanoscale*, 6(6):3083–3096, 2014.

[12] Zhe Zhang, Jan-Michael Y Carrillo, Suk-kyun Ahn, Bin Wu, Kunlun Hong, Gregory S Smith, and Changwoo Do. Atomistic structure of bottlebrush polymers: Simulations and neutron scattering studies. *Macromolecules*, 47(16):5808–5814, 2014.

[13] Jing Zhou, Sara A Turner, Sarah M Brosnan, Qiaoxi Li, Jan-Michael Y Carrillo, Dmytro Nykypanchuk, Oleg Gang, Valerie S Ashby, Andrey V Dobrynin, and Sergei S Sheiko. Shapeshifting: reversible shape memory in semicrystalline elastomers. *Macromolecules*, 47(5):1768–1776, 2014.

[14] Suk-kyun Ahn, Deanna L Pickel, W Michael Kochemba, Jihua Chen, David Uhrig, Juan Pablo Hinestrosa, Jan-Michael Y Carrillo, Ming Shao, Changwoo Do, Jamie M Messman, W Michael Brown, Bobby G Sumpter, and S Michael Kilbey. Poly (3-hexylthiophene) molecular bottlebrushes via ring-opening metathesis polymerization: macromolecular architecture enhanced aggregation. *ACS Macro Letters*, 2(8):761–765, 2013.

[15] Jan-Michael Y Carrillo, Rajeev Kumar, Monojoy Goswami, Bobby G Sumpter, and W Michael Brown. New insights into the dynamics and morphology of p3ht: Pcbm active layers in bulk heterojunctions. *Physical Chemistry Chemical Physics*, 15(41):17873–17882, 2013.

[16] Jan-Michael Y Carrillo, Fred C MacKintosh, and Andrey V Dobrynin. Nonlinear elasticity: from single chain to networks and gels. *Macromolecules*, 46(9):3679–3692, 2013.

[17] Sergei S Sheiko, Jing Zhou, Jamie Arnold, Dorota Neugebauer, Krzysztof Matyjaszewski, Constantinos Tsitsilianis, Vladimir V Tsukruk, Jan-Michael Y Carrillo, Andrey V Dobrynin, and Michael Rubinstein. Perfect mixing of immiscible macromolecules at fluid interfaces. *Nature materials*, 12(8):735–740, 2013.

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[19] Jan-Michael Y Carrillo and Andrey V Dobrynin. Contact mechanics of nanoparticles. *Langmuir*, 28(29):10881–10890, 2012.

[20] Jan-Michael Y Carrillo and Andrey V Dobrynin. Dynamics of nanoparticle adhesion. *The Journal of chemical physics*, 137(21):214902, 2012.

[21] Jan-Michael Y Carrillo, W Michael Brown, and Andrey V Dobrynin. Explicit solvent simulations of friction between brush layers of charged and neutral bottle-brush macromolecules. *Macromolecules*, 45(21):8880–8891, 2012.

[22] Trung Dac Nguyen, Jan-Michael Y Carrillo, Andrey V Dobrynin, and W Michael Brown. A case study of truncated electrostatics for simulation of polyelectrolyte brushes on gpu accelerators. *Journal of Chemical Theory and Computation*, 9(1):73–83, 2012.

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[23] Andrew J Oyer, Jan-Michael Y Carrillo, Chetan C Hire, Hannes C Schniepp, Alexandru D Asandei, Andrey V Dobrynin, and Douglas H Adamson. Stabilization of graphene sheets by a structured benzene/hexafluorobenzene mixed solvent. *Journal of the American Chemical Society*, 134(11):5018–5021, 2012.

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[25] Jan-Michael Y Carrillo and Andrey V Dobrynin. Layer-by-layer assembly of charged nanoparticles on porous substrates: molecular dynamics simulations. *ACS Nano*, 5(4):3010–3019, 2011.

[26] Jan-Michael Y Carrillo and Andrey V Dobrynin. Layer-by-layer assembly of polyelectrolyte chains and nanoparticles on nanoporous substrates: molecular dynamics simulations. *Langmuir*, 28(2):1531–1538, 2011.

[27] Jan-Michael Y Carrillo, Sergei S Sheiko, and Andrey V Dobrynin. Molecular dynamics simulations of bottlebrush macromolecules in two dimensional polymeric melts under flow conditions. *Soft Matter*, 7(6):2805–2811, 2011.

[28] Jan-Michael Y Carrillo and Andrey V Dobrynin. Polyelectrolytes in salt solutions: molecular dynamics simulations. *Macromolecules*, 44(14):5798–5816, 2011.

[29] Daniel Russano, Jan-Michael Y Carrillo, and Andrey V Dobrynin. Interaction between brush layers of bottle-brush polyelectrolytes: Molecular dynamics simulations. *Langmuir*, 27(17):11044–11051, 2011.

[30] Michael J Barrett, Frank C Sun, Alper Nese, Krzysztof Matyjaszewski, Jan-Michael Y Carrillo, Andrey V Dobrynin, and Sergei S Sheiko. Size separation of macromolecules during spreading. *Langmuir*, 26(19):15339–15344, 2010.

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[32] Jan-Michael Y Carrillo and Andrey V Dobrynin. Detailed molecular dynamics simulations of a model napss in water. *The Journal of Physical Chemistry B*, 114(29):9391–9399, 2010.

[33] Jan-Michael Y Carrillo and Andrey V Dobrynin. Effect of the electrostatic interactions on stretching of semiflexible and biological polyelectrolytes. *Macromolecules*, 43(5):2589–2604, 2010.

[34] Jan-Michael Y Carrillo and Andrey V Dobrynin. Molecular dynamics simulations of grafted layers of bottle-brush polyelectrolytes. *Langmuir*, 26(23):18374–18381, 2010.

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[36] Andrey V Dobrynin and Jan-Michael Y Carrillo. Universality in nonlinear elasticity of biological and polymeric networks and gels. *Macromolecules*, 44(1):140–146, 2010.

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[44] Daniel J Sandberg, Jan-Michael Y Carrillo, and Andrey V Dobrynin. Molecular dynamics simulations of polyelectrolyte brushes: From single chains to bundles of chains. *Langmuir*, 23(25):12716–12728, 2007.

Professional and Synergistic Activities

Membership	**American Physical Society (APS)**
Peer Reviewer	**American Physical Society (APS)**
	Physical Review Letters
Peer Reviewer	**American Chemical Society (ACS)**
	Macromolecules
	Macro Letters
	Industrial and Engineering Chemistry Research
Peer Reviewer	**Elsevier**
	Computational Materials Science
	International Journal of Solids and Structures
	Colloids and Surfaces A: Physicochemical and Engineering Aspects
Peer Reviewer	**Wiley**
	Macromolecular Theory and Simulations

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