Jan-Michael Y. Carrillo

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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*

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.

Research Experience

Oak Ridge National Laboratory/University of Tennessee Knoxville — **Oak Ridge, TN**
Research Scientist — *2015–Present*
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

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

Honors and Awards

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*

Selected Publications

U. Yamamoto, J.-M. Y. Carrillo, V. Bocharova, A. P. Sokolov, B. G. Sumpter, and K. S. Schweizer, "Theory and simulation of attractive nanoparticle transport in polymer melts," *Macromolecules*, vol. 51, no. 6, pp. 2258–2267, 2018.

B. Carroll, V. Bocharova, J.-M. Y. Carrillo, A. Kisliuk, S. Cheng, U. Yamamoto, K. S. Schweizer, B. G. Sumpter, and A. P. Sokolov, "Diffusion of sticky nanoparticles in a polymer melt: Crossover from suppressed to enhanced transport," *Macromolecules*, vol. 51, no. 6, pp. 2268–2275, 2018.

N. Jiang, M. K. Sen, W. Zeng, Z. Chen, J. Cheung, Y. Morimitsu, M. K. Endoh, T. Koga, M. Fukuto, G. Yuan, *et al.*, "Structure-induced switching of interpolymer adhesion at a solid-polymer melt interface," *Soft Matter*, vol. 14, no. 7, pp. 1108–1119, 2018.

W.-S. Xu, J.-M. Y. Carrillo, C. N. Lam, B. G. Sumpter, and Y. Wang, "Molecular dynamics investigation of the relaxation mechanism of entangled polymers after a large step deformation," *ACS Macro Letters*, vol. 7, no. 2, pp. 190–195, 2018.

J.-M. Y. Carrillo, J. Katsaras, B. G. Sumpter, and R. Ashkar, "A computational approach for modeling neutron scattering data from lipid bilayers," *Journal of Chemical Theory and Computation*, vol. 13, no. 2, pp. 916–925, 2017.

S. Cheng, S.-J. Xie, J.-M. Y. Carrillo, B. Carroll, H. Martin, P.-F. Cao, M. D. Dadmun, B. G. Sumpter, V. N. Novikov, K. S. Schweizer, *et al.*, "Big effect of small nanoparticles: A shift in paradigm for polymer nanocomposites," *ACS Nano*, vol. 11, no. 1, pp. 752–759, 2017.

S. Cheng, B. Carroll, W. Lu, F. Fan, J.-M. Y. Carrillo, H. Martin, A. P. Holt, N.-G. Kang, V. Bocharova, J. W. Mays, *et al.*, "Interfacial properties of polymer nanocomposites: Role of chain rigidity and dynamic heterogeneity length scale," *Macromolecules*, vol. 50, no. 6, pp. 2397–2406, 2017.

S. Cheng, B. Carroll, V. Bocharova, J.-M. Carrillo, B. G. Sumpter, and A. P. Sokolov, "Focus: Structure and dynamics of the interfacial layer in polymer nanocomposites with attractive interactions," *The Journal of Chemical Physics*, vol. 146, no. 20, p. 203201, 2017.

S.-k. Ahn, J.-M. Y. Carrillo, J. K. Keum, J. Chen, D. Uhrig, B. S. Lokitz, B. G. Sumpter, and S. M. Kilbey, "Nanoporous poly (3-hexylthiophene) thin film structures from self-organization of a tunable molecular bottlebrush scaffold," *Nanoscale*, vol. 9, no. 21, pp. 7071–7080, 2017.

J.-M. Y. Carrillo, M. E. Potter, M. A. Sakwa-Novak, S. H. Pang, C. W. Jones, and B. G. Sumpter, "Linking silica support morphology to the dynamics of aminopolymers in composites," *Langmuir*, vol. 33, no. 22, pp. 5412–5422, 2017.

A. Holewinski, M. A. Sakwa-Novak, J.-M. Y. Carrillo, M. E. Potter, N. Ellebracht, G. Rother, B. G. Sumpter, and C. W. Jones, "Aminopolymer mobility and support interactions in silica-pei composites for co2 capture applications: A quasielastic neutron scattering study," *The Journal of Physical Chemistry B*, vol. 121, no. 27, pp. 6721–6731, 2017.

Y. Han, J.-M. Y. Carrillo, Z. Zhang, Y. Li, K. Hong, B. G. Sumpter, M. Ohl, M. P. Paranthaman, G. S. Smith, and C. Do, "Thermoreversible morphology and conductivity of a conjugated polymer network embedded in block copolymer self-assemblies," *Small*, vol. 12, no. 35, pp. 4857–4864, 2016.

H.-H. Zhang, C. Ma, P. V. Bonnesen, J. Zhu, B. G. Sumpter, J.-M. Y. Carrillo, P. Yin, Y. Wang, A.-P. Li, and K. Hong, "Helical poly (5-alkyl-2, 3-thiophene) s: controlled synthesis and structure characterization," *Macromolecules*, vol. 49, no. 13, pp. 4691–4698, 2016.

J.-M. Y. Carrillo, Z. Seibers, R. Kumar, M. A. Matheson, J. F. Ankner, M. Goswami, K. Bhaskaran-Nair, W. A. Shelton, B. G. Sumpter, and I. S. Michael Kilbey, "Petascale simulations of the morphology and the molecular interface of bulk heterojunctions," *ACS Nano*, 2016. ASAP, DOI:10.1021/acsnano.6b03009.

A. P. Martinez, J.-M. Y. Carrillo, A. V. Dobrynin, and D. H. Adamson, "Distribution of chains in polymer brushes produced by a "grafting from" mechanism," *Macromolecules*, vol. 49, no. 2, pp. 547–553, 2016.

J.-M. Y. Carrillo, M. A. Sakwa-Novak, A. Holewinski, M. E. Potter, G. Rother, C. W. Jones, and B. G. Sumpter, "Unraveling the dynamics of aminopolymer/silica composites," *Langmuir*, vol. 32, no. 11, pp. 2617–2625, 2016.

S. Cheng, S. Mirigian, J.-M. Y. Carrillo, V. Bocharova, B. G. Sumpter, K. S. Schweizer, and A. P. Sokolov, "Revealing spatially heterogeneous relaxation in a model nanocomposite," *The Journal of Chemical Physics*, vol. 143, no. 19, p. 194704, 2015.

Z. Cao, J.-M. Y. Carrillo, S. S. Sheiko, and A. V. Dobrynin, "Computer simulations of bottle brushes: From melts to soft networks," *Macromolecules*, vol. 48, no. 14, pp. 5006–5015, 2015.

J.-M. Y. Carrillo, S. Cheng, R. Kumar, M. Goswami, A. P. Sokolov, and B. G. Sumpter, "Untangling the effects of chain rigidity on the structure and dynamics of strongly adsorbed polymer melts," *Macromolecules*, vol. 48, no. 12, pp. 4207–4219, 2015.

W. M. Brown, J.-M. Y. Carrillo, N. Gavhane, F. M. Thakkar, and S. J. Plimpton, "Optimizing legacy molecular dynamics software with directive-based offload," *Computer Physics Communications*, vol. 195, pp. 95–101, 2015.

Z. Cao, M. J. Stevens, J.-M. Y. Carrillo, and A. V. Dobrynin, "Adhesion and wetting of soft nanoparticles on textured surfaces: Transition between wenzel and cassie–baxter states," *Langmuir*, vol. 31, no. 5, pp. 1693–1703, 2015.

S. J. Woltornist, J.-M. Y. Carrillo, T. O. Xu, A. V. Dobrynin, and D. H. Adamson, "Polymer/pristine graphene based composites: From emulsions to strong, electrically conducting foams," *Macromolecules*, vol. 48, no. 3, pp. 687–693, 2015.

S.-k. Ahn, J.-M. Y. Carrillo, Y. Han, T.-H. Kim, D. Uhrig, D. L. Pickel, K. Hong, S. M. Kilbey, B. G. Sumpter, G. S. Smith, and C. Do, "Structural evolution of polylactide molecular bottlebrushes: Kinetics study by size exclusion chromatography, small angle neutron scattering, and simulations," *ACS Macro Letters*, vol. 3, no. 9, pp. 862–866, 2014.

J.-M. Y. Carrillo and A. V. Dobrynin, "Salt effect on osmotic pressure of polyelectrolyte solutions: Simulation study," *Polymers*, vol. 6, no. 7, pp. 1897–1913, 2014.

J.-M. Y. Carrillo and B. G. Sumpter, "Structure and dynamics of confined flexible and unentangled polymer melts in highly adsorbing cylindrical pores," *The Journal of Chemical Physics*, vol. 141, no. 7, p. 074904, 2014.

T. D. Nguyen, J.-M. Y. Carrillo, M. A. Matheson, and W. M. Brown, "Rupture mechanism of liquid crystal thin films realized by large-scale molecular simulations," *Nanoscale*, vol. 6, no. 6, pp. 3083–3096, 2014.

Z. Zhang, J.-M. Y. Carrillo, S.-k. Ahn, B. Wu, K. Hong, G. S. Smith, and C. Do, "Atomistic structure of bottlebrush polymers: Simulations and neutron scattering studies," *Macromolecules*, vol. 47, no. 16, pp. 5808–5814, 2014.

J. Zhou, S. A. Turner, S. M. Brosnan, Q. Li, J.-M. Y. Carrillo, D. Nykypanchuk, O. Gang, V. S. Ashby, A. V. Dobrynin, and S. S. Sheiko, "Shapeshifting: reversible shape memory in semicrystalline elastomers," *Macromolecules*, vol. 47, no. 5, pp. 1768–1776, 2014.

S.-k. Ahn, D. L. Pickel, W. M. Kochemba, J. Chen, D. Uhrig, J. P. Hinestrosa, J.-M. Y. Carrillo, M. Shao, C. Do, J. M. Messman, W. M. Brown, B. G. Sumpter, and S. M. Kilbey, "Poly (3-hexylthiophene) molecular bottlebrushes via ring-opening metathesis polymerization: macromolecular architecture enhanced aggregation," *ACS Macro Letters*, vol. 2, no. 8, pp. 761–765, 2013.

J.-M. Y. Carrillo, R. Kumar, M. Goswami, B. G. Sumpter, and W. M. Brown, "New insights into the dynamics and morphology of p3ht: Pcbm active layers in bulk heterojunctions," *Physical Chemistry Chemical Physics*, vol. 15, no. 41, pp. 17873–17882, 2013.

J.-M. Y. Carrillo, F. C. MacKintosh, and A. V. Dobrynin, "Nonlinear elasticity: from single chain to networks and gels," *Macromolecules*, vol. 46, no. 9, pp. 3679–3692, 2013.

S. S. Sheiko, J. Zhou, J. Arnold, D. Neugebauer, K. Matyjaszewski, C. Tsitsilianis, V. V. Tsukruk, J.-M. Y. Carrillo, A. V. Dobrynin, and M. Rubinstein, "Perfect mixing of immiscible macromolecules at fluid interfaces," *Nature Materials*, vol. 12, no. 8, pp. 735–740, 2013.

S. J. Woltornist, A. J. Oyer, J.-M. Y. Carrillo, A. V. Dobrynin, and D. H. Adamson, "Conductive thin films of pristine graphene by solvent interface trapping," *ACS Nano*, vol. 7, no. 8, pp. 7062–7066, 2013.

T. D. Nguyen, J.-M. Y. Carrillo, A. V. Dobrynin, and W. M. Brown, "A case study of truncated electrostatics for simulation of polyelectrolyte brushes on gpu accelerators," *Journal of Chemical Theory and Computation*, vol. 9, no. 1, pp. 73–83, 2012.

Full Publication List and ORCID

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

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

`http://www.researcherid.com/rid/K-7170-2013`

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