

CURRICULUM VITAE

Wang, Jian-Sheng

Personal Particulars

Date of Birth: 8 February 1960
 Place of Birth: Nei Monggol, China
 Citizenship: Singapore citizen
 Address: Department of Physics,
 National University of Singapore,
 2 Science Drive 3, Singapore 117551.
 Tel: +65 6516 6880
 E-mail: phywjs@nus.edu.sg
<https://www.physics.nus.edu.sg/~phywjs/>
 ResearcherID: A-1758-2012
 Scopus author ID: 16437835600
 ORCID: <http://orcid.org/0000-0002-5119-8382>
<https://scholar.google.com.sg/citations?user=Dc7akeoAAAAJ>

Field of Research

Computational statistical and condensed matter physics. Earlier, phase transitions, cluster Monte Carlo algorithms, efficient Monte Carlo techniques. Nonequilibrium Green's function (NEGF) method, quantum master equations, nanostructures and thermal and electronic transport, transport in oxides. Also, most recently, ultra-near-field radiative heat transfer using NEGF.

Education and Experience

- Tumu Er Tai High School, 1977, Chayou Houqi, Nei Monggol, China
- B. Sc. January 1982, Jilin University, Changchun, Jilin Province, China
- CUSPEA 1982, top 34th
- M. Sc. May 1984, Carnegie-Mellon University, Pittsburgh, Pennsylvania, U. S. A.
- Ph. D. August 1987, Carnegie-Mellon University, Pittsburgh, Pennsylvania, U. S. A.
- Supercomputer Postdoctoral Fellow, August 1987 – February 1989, Rutgers University, U. S. A.
- Research Scientist, March 1989 – February 1990, HLRZ, Jülich, Germany
- Postdoctoral Fellow, March 1990 – August 1991, Max-Planck-Institut für Polymerforschung and Universität Mainz, Germany
- Lecturer, September 1991 – May 1993, Hong Kong Baptist College, Hong Kong
- Lecturer, June 1993; Senior Lecturer, July 1995; Associate Professor, August 1998; Professor July 2005, Department of Computational Science, National University of Singapore
- Acting Head, Department of Computational Science, National University of Singapore, November 1999 – December 2000
- Deputy Head, Department of Computational Science, National University of Singapore, July 2002 – December 2003
- Adjunct appointment, Institute of High Performance Computing, April 2006 – March 2010
- Deputy Head (Research), Department of Physics, July 2010 – June 2017
- Provost's Chair, July 2014 – June 2017

Services/Recognition

- Long Service Medal - National Day Awards 2018.
- Institute of Physics Singapore ‘World Scientific Award,’ 2017.
- Fellow of the American Physical Society, 2005.
- Member of the American Physical Society, 1986-1989, and 1997 - 2020.
- Fellow of Singapore-MIT Alliance, 1999-2010.
- Member of Local Organizing Committee of ICCP4, Singapore, June 1997.
- Member of Scientific Committee of VECPAR’96, 98, and 2000, Porto, Portugal.
- Member of International Advisory Committees of Statphys21, Cancun, Mexico, July 2001; Statphys22, Bangalore, India, July 2004; Statphys23, Genova, Italy, July 2007; Statphys24, Cairns, Australia, July 2010; Statphys25, Seoul, Korea, 2013, Statphys26, Lyon, France, July 2016; Statphys27, Buenos Aires, Argentina 2019; Statphys28, Tokyo, Japan, August 2022.
- Member of International Advisory Committee of CCP2001, Aachen, Germany, September 2001; CCP2009, Kaohsiung, Taiwan, December 2009; CCP2010, Trondheim, Norway, June 2010; CCP2011, Gatlinburg, Tennessee, USA, November 2011; CCP2015, IIT Guwahati, India, December 2015.
- Member of the Commission on Computational Physics (IUPAP C20), Nov 2008 – Oct 2011.
- Member of Scientific Programme Committee of MCQMC2002, Singapore, December 2002.
- Member of International Advisory Committee of StatPhys-Taiwan-2002, May 2002.
- Member of Local Organizing Committee, ICMAT 2003, Symposium K, theory, modeling, and simulation, Singapore, 7-12 December 2003.
- Co-chair, Markov Chain Monte Carlo workshop, Institute of Mathematical Sciences (IMS), Singapore, 1-28 March 2004; also co-editor of the proceedings: IMS lecture notes series, volume 7, World Scientific, 2005.
- Member of International Organizing Committee, the 1st international workshop on simulational physics, Hangzhou, 5-7 November 2004. Also an invited speaker.
- Judge (open category), HPC Quest 2004.
- Guest Professor, Huazhong University of Science and Technology, May 2004 - May 2006.
- On the Editorial Board, International Journal of Modern Physics C, World Scientific, 2005 - .
- On the Editorial Board, Phase Transitions, Taylor & Francis, 2010 - .
- On the Editorial Board, Entropy, MDPI, 2020 - .
- Associate Editor of the European Physical Journal B, 2010 - 2019.
- Member of the Scientific Committee of the AAPPS Bulletin, 2019 - .
- Member of Faculty Promotion and Tenure Committee (Senior), July 2008 – June 2012.
- On the OCPA8 Organization Committee of the topic session of Computational and Mathematical Physics, June 2014.
- Referee for “Physical Review Letters,” “Physical Review E,” “Journal of Statistical Physics,” “Physica A,” “Europhysics Letters,” “Journal of Physics: condensed matter”, “Modern Physics Letters B,” and “Computational Materials Science.”
- Research grant reviewing for National Science and Technology Board (now A*star), Research Grants Council of Hong Kong, and National Science Foundation (USA).

Invited Talks on International Conferences and Workshops

- Workshop on Fermion Algorithms, 10–12 April 1991, HLRZ, Jülich, Germany.
- Asian Conference on Computer Vision (ACCV’95), 5–8 December 1995, Singapore.
- Computational Physics Workshop, 27–29 May 1996, Univ of Tokyo, Japan.
- Polymer Processing towards AD2000, 26–28 November 1996, Singapore.
- Hong Kong Workshop on Computational Physics, 9–20 June 1997, Chinese Univ.

- Statphys-Taipei-1997, 3–11 August 1997, Academia Sinica, Taipei, Taiwan.
- Workshop on Computational Materials Science and Biology, 8–12 June 1998, Beijing International Center for Computational Physics.
- Workshop on Statistical and Computational Physics, 25–27 June 1998, Academia Sinica, Taiwan.
- The EPS-IUPAP-IOP Conference on Computational Physics (CCP98), 2–5 September 1998, Granada, Spain.
- APS Centennial/CCP99, 20–26 March 1999, Atlanta, Georgia, USA.
- International Topical Symposium on Statistical Physics (Statphys-Taiwan-1999), 8–16 August 1999, Academia Sinica, Taiwan.
- The 5th International Conference on Computational Physics (ICCP5), 11–13 October 1999, Kanazawa, Japan.
- The 3rd Joint Meeting of Chinese Physicists World-Wide, 31 July – 4 August 2000, Hong Kong.
- 4th International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing (MCQMC 2000), 27 November – 1 December 2000, Hong Kong.
- Fourteenth Workshop on “Computer Simulation Studies in Condensed Matter Physics,” 19-24 February 2001, Athens, Georgia, USA.
- Workshop on Novel Ordering and Phase Transitions, 10–12 June 2002, Kyoto, Japan.
- The First Cross-Strait Conference on Statistical Physics, 27–31 August 2003, Yangzhou, China.
- The Monte Carlo Method in the Physical Sciences: celebrating the 50th anniversary of the Metropolis algorithm, 9–11 June 2003, Los Alamos, USA.
- Workshop on “Monte Carlo Methods in Scientific Computing”, 3–7 November 2003, Beijing, China.
- 2nd Asia-Pacific Physics Workshop (Frontier in Condensed Matter Physics), 21–24 June 2004, Hong Kong, China.
- Statistical Physics of Disordered Systems and Its Applications, 12–15 July 2004, Shonan Village Center, Hayama, Japan.
- 13th Condensed-Matter and StatPhys Meeting, 25–27 August 2005, Yichuan, China.
- Frontiers in Computational Methods and Their Applications in Physical Sciences, 6–13 December 2005, Chinese University of Hong Kong.
- International Conference on the Frontiers of Nonlinear and Complex Systems, 24–26 May 2006, Hong Kong Baptist University, Hong Kong.
- CCP2006-Korea, 29 August – 1 September, 2006, Gyeongju, Korea.
- TIENCS 4–6 June 2008, and TIENCS 5–9 July 2010, Singapore.
- Danish Physical Society Nordic Meeting, 16–18 June 2009, Lyngby, Denmark.
- The 6th Joint Meeting of Chinese Physicists Worldwide International Conference on Physical Education and Frontier Physics (OCPA6), 3–7 August 2009, Lanzhou, China.
- APCTP Workshop on Current Progress of Simulations in Complex Systems, 15–17 November 2010, Pohang, Korea.
- Multiscale Modeling, Simulation, Analysis and Applications, 19–21 December 2011, Institute for Mathematical Sciences, Singapore.
- Advanced Workshop on Energy Transport in Low-Dimensional Systems, 15–24 October 2012, Trieste, Italy.
- The 1st International Conference on Phononics and Thermal Energy Science (PTES2013), 26 August – 4 September 2013, Shanghai, China.
- 27th Annual ‘Center for Simulational Physics’ Workshop, 24-28 February, 2014, University of Georgia, USA.
- Chinese Physical Society fall meeting, 12-14 September 2014, Harbin, China.
- The 1st conference on condensed matter physics, 15-17 July 2015, Tsinghua University, Beijing, China.
- Conference on Computational Physics (CCP2015), 2-5 December 2015, IIT Guwahati, India.

- Workshop ‘Towards reality in modelling of molecular electronics,’ 13-17 June 2016, San Sebastian, Spain.
- Workshop ‘Generalised Langevin equation: theory & applications,’ 12-13 January 2017, King’s College London, UK.
- Phonons & PTES 2018, 30 May - 3 June 2018, Nanjing, China.
- Lectures at CSRC Summer School on ‘Quantum non-equilibrium Phenomena: methods and applications,’ 17-21 June 2019, Beijing, China.
- 5th ‘Statistical Physics and Complex Systems Conference’, 26-29 July 2019, USTC, Hefei, China (plenary talk).
- WTT2020, Qingdao, Nov 2020, China.
- IBS Colloquium talk, 24 March 2021, South Korea.
- 16th Granada seminar, 7-17 June 2021, Spain.

Students and Postdocs

- M.Sc.

Zhan Zhifang 1998-2000, Lee Lik Wee 1999-2000, Cheng Siew Yen 1999-2000, Qu Zhengping 1999-2000, Sugiarto Radjiman 2003-2005, Luo Jie 2004-2006, Imam Makfudz 2007-2009, Janakiraman Balachandran 2007-2009, Siu Zhuo Bin 2008-2010, Zhang Li 2014 - 2016, Xu Xiansong 2016 - 2017.

- Ph.D.

Zeng Nan 2004-2006, Ni Xiaoxi 2007-20011, Zhang Lifa 2007-2011, Leek Meng Lee 2008-2012, Bijay Kumar Agarwalla 2008-2013, Thingna Juzar Yahya 2008-2012, Li Huanan 2009-2013, Zhou Hangbo 2011-2016, Qiu Hongfei 2012-2017, Chen Ruofan 2013-2017, Peng Jiebin 2015-2017, Yap Han Hoe 2016 -2020, Sun Kangtai 2017 -2021.

- Postdocs

Gerald G. Pereira 1996-1997, Lin Yi 2000-2002, Jun Cai 2001-2002, Jian Wang 2005-2007, Jing-Tao Lü 2007-2008, Eduardo Chaves Cuansing Jr 2008-2010, Jinwu Jiang 2008-2011, Ren Jichang 2015-2018, Yang Kaike 2016 - 2017, Tang Gaomin 2018 - 2019, Zhu Tao 2019 - 2022, Zhang Zuquan 2019 - 2022, Gao Zhibin 2019 - 2021.

Grants

- ARC, S\$363,700, 1/1998-12/2001, “Computational nano-science programme.”
- FRC, S\$112,500, 7/2003 - 7/2006, “Transport phenomena in nanostructure.”
- FRC tier 1, S\$166,400, 7/2006 - 9/2009, “Heat transport in mesoscopic systems.”
- URC tier 1, S\$250,000, 6/2009 - 5/2012, “Phonons and interactions with quasiparticles.”
- FRC tier 1, S\$170,000, 1/2015 - 12/2017, “First principles prediction of the thermoelectric figure of merit ZT.”
- MOE tier 2, S\$662,000, 5/2015 - 4/2018. “Oxide thermoelectrics: theory and experiment.”
- MOE tier 2, S\$462,000, 1/2019-12/2021. “Energy transport in the near field.”

Research Contribution and Impact

I did pioneering work in cluster algorithms and in replica Monte Carlo simulation. I proposed flat-histogram algorithm, and perfected transition matrix Monte Carlo method. In addition, I did original and significant work in spin glasses, nonequilibrium driven diffusive systems, and random sequential adsorptions. My recent interests have been in quantum thermal transport in nanostructures, with an emphasis on the nonequilibrium Green’s function (NEGF) method. In addition, I’m interested in Boltzmann equation approach to transport, applying to perovskite oxides. Most recently, I focus on near-field radiative heat transfer.

- The most cited and best known work is the Swendsen-Wang algorithm for the Monte Carlo simulation of Ising and Potts models [paper number 2 in the list of publications, 2040 WoS citations]. This algorithm is nothing like the previously known Monte Carlo algorithms (such as single-spin-flip

Metropolis algorithm) which are based on local moves. In fact, the Swendsen-Wang algorithm opens up a whole new area of research for nonlocal updating algorithms, also known as cluster algorithms. The advantage of the cluster algorithms over the local updating is much reduced critical slowing down. Thus the algorithm is most effective and efficient at second order phase transitions. The cluster algorithm is used widely in high-precision simulation works. This algorithm has become a standard example of efficient Monte Carlo sampling, and is discussed in many textbooks and monographs [e.g., Heermann (1990), “Computer Simulation Methods,” 2nd ed, p.91; Frenkel & Smit (1996), “Understanding Molecular Simulation,” ch. 12; Thijssen (1999), “Computational Physics,” p.393; Newman & Barkema (1999), “Monte Carlo Methods in Statistical Physics,” ch.4.4.1; Landau & Binder, “A Guide to Monte Carlo Simulations in Statistical Physics,” p.134; Liu (2001), “Monte Carlo Strategies in Scientific Computing,” ch.7; Rubinstein & Kroese (2008), “Simulation and the Monte Carlo Method,” 2nd ed, p.180]. It is fair to say that it is a great breakthrough in Monte Carlo simulation methods in decades. The method is generalized in dozen ways for a variety of systems, such as continuous spin systems, vertex models, field-theoretic models, quantum systems, fluid mixtures, etc. Its application domain has gone beyond statistical physics to image processing, computer science, and statistics.

- (b) Swendsen and I have also developed an algorithm known as replica Monte Carlo [paper number 1, with 1230 citations] specially designed for spin glasses. This algorithm is one of the earliest cluster algorithms (unrelated to the Swendsen-Wang algorithm), and it is one of the earliest algorithms that uses multiple systems (at different temperatures). The later replica-exchange algorithm and simulated tempering can find their root from our seemingly sophisticated method. People have paid more attentions to this algorithm in recent years in biophysics and other field.
- (c) In nonequilibrium statistical mechanics, I discovered an unusual long-range correlation in driven lattice gas system at high temperatures. This work, done together with Zhang, Lebowitz, and Valles, has led to further development [paper number 7]. I also made the most extensive Monte Carlo simulation studies of the phase transitions in such systems, clarifying some of long-standing controversies (such as the location of the critical temperature T_c and the validity of anisotropic finite-size scaling) [paper number 38 and 52].
- (d) In the studies of random sequential adsorption (RSA), my most important contribution is a discovery of a quantitative relation between the RSA model and a corresponding equilibrium system in terms of graphs of Mayer expansion. Various aspects of RSA are studied. Comprehensive results, including high precision jamming coverage in event-driven simulation and computer-aided series expansions, are summarized in a review article [paper number 56].
- (e) Additional contribution to the simulation techniques is an algorithm, known as flat-histogram algorithm, to generate samples with a uniform probability distribution in energy, as oppose to canonical distribution. This sampling method has connection with the broad histogram method of Oliveira, multi-canonical ensemble of Berg et al, and entropy sampling of Lee. Together with a data analysis method known as transition matrix Monte Carlo, the simulation technique is a tool generalized the previous methods and is more accurate. This method gives a good way of evaluating the thermodynamic free energy for all values of temperatures from a single Monte Carlo simulation run [paper number 53, and 67]. Unfortunately, this method is overshadowed by a simpler but more powerful method known as “Wang-Landau” method.
- (f) In the most recent years, my research interests shifted away from Monte Carlo and focused on thermal transport problems. With Baowen Li, I showed that the exponent $1/3$ is generic for the divergence of heat conductivity with chain lengths for models with transverse motions [paper number 90, 92]. I developed quantum heat transport theory based on nonequilibrium Green’s function formalism [paper number 103, 112, 189]. This theory is applied to variety of systems of practical importance, such as carbon nanotubes and graphene sheets. It is also applied to many interesting problems, such as quantum thermal rectification, phonon Hall effect, full counting statistics of energy transport. A review article, paper number 112, is well-read, and has received 431 citations. The most recent effort in research is the application of NEGF to thermal radiation involving (scalar) photons. I also look into angular momentum transfer and Casimir force.

Books

- “Markov Chain Monte Carlo: innovations and applications,” W. S. Kendall, F. Liang, and J.-S. Wang, editors, World Scientific (2005).
- “Advanced Statistical Mechanics,” J.-S. Wang, World Scientific (2022).

LIST OF PUBLICATIONS

1. R. H. Swendsen and J.-S. Wang, “Replica Monte Carlo simulation of spin glasses,” *Phys. Rev. Lett.* **57**, 2607 (1986).
2. R. H. Swendsen and J.-S. Wang, “Nonuniversal critical dynamics in Monte Carlo simulations,” *Phys. Rev. Lett.* **58**, 86 (1987).
3. J.-S. Wang and R. H. Swendsen, “Monte Carlo renormalization-group study of Ising spin glasses,” *Phys. Rev. B* **37**, 7745 (1988).
4. J.-S. Wang and R. H. Swendsen, “Low-temperature properties of the $\pm J$ Ising spin glass in two dimensions,” *Phys. Rev. B* **38**, 4840 (1988).
5. J.-S. Wang and R. H. Swendsen, “Monte Carlo and high-temperature-expansion calculations of a spin-glass effective Hamiltonian,” *Phys. Rev. B* **38**, 9086 (1988).
6. J.-S. Wang and J. L. Lebowitz, “Phase transitions and universality in nonequilibrium steady states of stochastic Ising models,” *J. Stat. Phys.* **51**, 893 (1988).
7. M. Q. Zhang, J.-S. Wang, J. L. Lebowitz, and J. L. Vallés, “Power law decay of correlations in stationary nonequilibrium lattice gases with conservative dynamics,” *J. Stat. Phys.* **52**, 1461 (1988).
8. K. Binder and J.-S. Wang, “Finite-size effects at critical points with anisotropic correlations—phenomenological scaling theory and Monte Carlo simulations,” *J. Stat. Phys.* **55**, 87 (1989).
9. J.-S. Wang, K. Binder, and J. L. Lebowitz, “Computer simulation of driven diffusive systems with exchanges,” *J. Stat. Phys.* **56**, 783 (1989).
10. J.-S. Wang, R. H. Swendsen, and R. Kotecký, “Antiferromagnetic Potts models,” *Phys. Rev. Lett.* **63**, 109 (1989).
11. J.-S. Wang and D. Chowdhury, “The critical behaviour of the three-dimensional dilute Ising model: universality and the Harris criterion,” *J. Phys. France* **50**, 2905 (1989).
12. J.-S. Wang, “Clusters in the three-dimensional Ising model with a magnetic field,” *Physica A* **161**, 249 (1989).
13. J.-S. Wang and D. Stauffer, “Fractal dimension of 3D Ising droplets,” *Z. Phys. B* **78**, 145 (1990).
14. J.-S. Wang, W. Selke, Vl. S. Dotsenko, and V. B. Andreichenko, “The two-dimensional random-bond Ising model at criticality—a Monte Carlo study,” *Europhys. Lett.* **11**, 301 (1990).
15. J.-S. Wang, W. Selke, Vl. S. Dotsenko, and V. B. Andreichenko, “The critical behavior of the two-dimensional dilute Ising magnet,” *Physica A* **164**, 221 (1990).
16. J.-S. Wang, “Critical dynamics of the Swendsen-Wang algorithm in the three-dimensional Ising model,” *Physica A* **164**, 240 (1990).
17. J.-S. Wang, M. Wöhlert, H. Mühlenbein, and D. Chowdhury, “The three-dimensional dilute Ising model,” *Physica A* **166**, 173 (1990).
18. J.-S. Wang, R. H. Swendsen, and R. Kotecký, “Three-state antiferromagnetic Potts models: A Monte Carlo study,” *Phys. Rev. B* **42**, 2465 (1990).
19. V. B. Andreichenko, Vl. S. Dotsenko, W. Selke, and J.-S. Wang, “Monte Carlo study of the 2D Ising model with impurities,” *Nucl. Phys. B* **344**, 531 (1990).
20. J.-S. Wang and R. H. Swendsen, “Cluster Monte Carlo algorithms,” *Physica A* **167**, 565 (1990).
21. T. S. Ray and J.-S. Wang, “Metastability and nucleation in Ising models with Swendsen-Wang dynamics,” *Physica A* **167**, 580 (1990).
22. P. Nielaba, V. Privman, and J.-S. Wang, “Kinetics of multilayer adsorption: Monte Carlo studies of models without screening,” *J. Phys. A: Math. Gen.* **23**, L1187 (1990).

23. V. Privman, J.-S. Wang, and P. Nielaba, "Continuum limit in random sequential adsorption," *Phys. Rev. B* **43**, 3366 (1991).
24. R. Dickman, J.-S. Wang, and I. Jensen, "Random sequential adsorption: series and virial expansions," *J. Chem. Phys.* **94**, 8252 (1991).
25. R. Hilfer and J.-S. Wang, "Analysis of multilayer adsorption models without screening," *J. Phys. A: Math. Gen.* **24**, L389 (1991).
26. J.-S. Wang and K. Binder, "Wetting transitions in polymer blends: A Monte Carlo lattice simulation," *J. Chem. Phys.* **94**, 8537 (1991).
27. J.-S. Wang and K. Binder, "Enrichment of the chain ends in polymer melts at interfaces," *J. Phys. I France*, **1**, 1583 (1991).
28. R. H. Swendsen, J.-S. Wang, and A. M. Ferrenberg, "New Monte Carlo methods for improved efficiency of computer simulations in statistical mechanics," in *The Monte Carlo Method in Condensed Matter Physics*, ed. K. Binder, (Springer, Berlin), Topics in Applied Physics Vol 71, p. 75, (1992).
29. J.-S. Wang, "Cluster Monte Carlo algorithms in statistical mechanics," proceedings of the 'Workshop on Fermion Algorithms,' *Int. J. Mod. Phys. C* **3**, 209 (1992).
30. J.-S. Wang and K. Binder, "Chain linear dimensions in the surface-enriched layer of polymer mixtures," *Makromol. Chem., Theory Simul.* **1**, 49 (1992).
31. V. Privman and J.-S. Wang, "Asymptotic layer coverage in deposition models without screening," *Phys. Rev. A* **45**, R2155 (1992).
32. J.-S. Wang, P. Nielaba, and V. Privman, "Collective effects in random sequential adsorption of diffusing hard squares," *Mod. Phys. Lett. B* **7**, 189 (1993).
33. P. Nielaba, V. Privman, and J.-S. Wang, "Irreversible multilayer adsorption," in *Computer Simulation Studies in Condensed-Matter Physics VI*, D. P. Landau, K. K. Mon, H.-B. Schüttler, eds., Springer Proceedings in Physics, Vol. 76, p. 143 (Springer-Verlag, Berlin, 1993).
34. J.-S. Wang, P. Nielaba, and V. Privman, "Locally frozen defects in random sequential adsorption with diffusional relaxation," *Physica A* **199**, 527 (1993).
35. P. Nielaba, V. Privman, and J.-S. Wang, "Irreversible multilayer adsorption," in the proceedings *Phase Transitions at Interfaces*, *Berichte der Bunsengesellschaft für Physikalsche Chemie*, **98**, 451 (1994).
36. J.-S. Wang, "A fast algorithm for random sequential adsorption of discs," *Int. J. Mod. Phys. C* **5**, 707 (1994).
37. A. Esser, V. Dohm, M. Hermes, J.-S. Wang, "Field theory of finite-size effects in Ising-like systems," *Z. Phys. B* **97**, 205 (1995).
38. J.-S. Wang, "Anisotropic finite-size scaling analysis of a two-dimensional driven diffusive system," *J. Stat. Phys.* **82**, 1409 (1996).
39. R. K. Heilmann, J.-S. Wang, and R. H. Swendsen, "Rotationally symmetric ordered phase in the three-state antiferromagnetic Potts model," *Phys. Rev. B* **53**, 2210 (1996).
40. J.-S. Wang, "Cluster Monte Carlo algorithms and their applications," in *Recent Developments in Computer Vision (ACCV'95 Invited Session Papers)*, S. Z. Li, D. P. Mital, E. K. Teoh, and H. Wang, Eds., Lecture Notes in Computer Science – 1035, p. 307 (Springer-Verlag, Berlin, 1996).
41. G. G. Pereira and J.-S. Wang, "A Monte Carlo study of wetting transitions in polymer blends confined to a capillary," *J. Chem. Phys.* **104**, 5294 (1996).
42. C.-K. Gan and J.-S. Wang, "An algorithm for series expansions based on hierarchical rate equations," *J. Phys. A: Math. Gen.* **29**, L177 (1996).
43. G. G. Pereira and J.-S. Wang, "Effect of van der Waals surface interactions on wetting transitions in polymer blends," *Phys. Rev. E* **54**, 3040 (1996).

44. G. G. Pereira and J.-S. Wang, "Wetting transitions in polymer blends: comparison between simulation and theory," *J. Chem. Phys.* **105**, 3849 (1996).
45. J.-S. Wang and R. B. Pandey, "Kinetics and jamming coverage in a random sequential adsorption of polymer chains," *Phys. Rev. Lett.* **77**, 1773 (1996).
46. C. K. Gan and J.-S. Wang, "Series-expansion studies of random sequential adsorption with diffusional relaxation," *Phys. Rev. E* **55**, 107 (1997).
47. G. G. Pereira and J.-S. Wang, "Effect of diffusional relaxation in random sequential adsorption of polymer chains," *Physica A* **242**, 347 (1997).
48. C. K. Gan and J.-S. Wang, "Extended series expansions for random sequential adsorption," *J. Chem. Phys.* **108**, 3010 (1998).
49. J.-S. Wang and C. K. Gan, "Nonequilibrium relaxation of the two-dimensional Ising model: series-expansion and Monte Carlo studies," *Phys. Rev. E* **57**, 6548 (1998).
50. J.-S. Wang, "Random sequential adsorption, series expansion and Monte Carlo simulation," *Physica A* **254**, 179 (1998).
51. J.-S. Wang, "Ising relaxation dynamics, series expansions and Monte Carlo simulations," in *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, Vol XI, p.125, D. P. Landau and H. B. Schuettler, eds., (Springer-Verlag, 1999).
52. K.-t. Leung and J.-S. Wang, "Anisotropic finite-size scaling analysis of a three-dimensional driven-diffusive system," *Int. J. Mod. Phys. C* **10**, 853 (1999).
53. J.-S. Wang, T. K. Tay, and R. H. Swendsen, "Transition matrix Monte Carlo reweighting and dynamics," *Phys. Rev. Lett.* **82**, 476 (1999).
54. J.-S. Wang, "Transition matrix Monte Carlo method," CCP98 conference proceedings, *Comp. Phys. Commu.* **121-122**, 22 (1999).
55. J.-S. Wang, "Is the broad histogram random walk dynamics correct?" *Eur. Phys. J. B* **8**, 287 (1999).
56. J.-S. Wang, "Series expansion and computer simulation studies of random sequential adsorption," special issue 'Adhesion of Submicron Particles on Solid Surfaces', *Colloids and Surfaces A* **165**, 325 (2000).
57. J.-S. Wang and L. W. Lee, "Monte Carlo algorithms based on the number of potential moves," CCP99 conference proceedings, *Comp. Phys. Commu.* **127**, 131 (2000).
58. R. H. Swendsen, B. Diggs, J.-S. Wang, S.-T. Li, C. Genovese, J. B. Kadane, "Transition matrix Monte Carlo," *Int. J. Mod. Phys. C* **10**, 1563 (1999).
59. J.-S. Wang, "Flat histogram Monte Carlo method," Statphys-Taiwan 1999 conference proceedings, *Physica A* **281**, 147 (2000).
60. J.-S. Wang, "Taylor series expansion and computer simulation studies of random sequential adsorption," ICCP5 conference proceedings, Kanazawa, Japan, *Prog. Theor. Phys. Suppl.* **138**, 433 (2000).
61. J.-S. Wang, "Flat histogram Monte Carlo method," ICCP5 conference proceedings, Kanazawa, Japan, *Prog. Theor. Phys. Suppl.* **138**, 454 (2000).
62. C.-P. Chng and J.-S. Wang, "Unequal intralayer coupling in a bilayer driven lattice gas," *Phys. Rev. E* **61**, 4962 (2000).
63. S. Y. Cheng, J.-S. Wang, and G. Xu, "Microstructural studies of organic light-emitting devices by Monte Carlo simulation of two-dimensional triangles," *Phys. Rev. B* **62**, 11405 (2000).
64. Z. F. Zhan, L. W. Lee, and J.-S. Wang, "A new approach to the study of the ground-state properties of 2D Ising spin glass," *Physica A* **285**, 239 (2000).
65. L. Yi and J.-S. Wang, "Conductance oscillations in interacting mesoscopic systems with multiple energy levels: quantum interference," *Phys. Rev. B* **63**, 073304 (2001).

66. J. Cai and J.-S. Wang, "Reconstruction of Si(001) and adsorption of Si adatoms and ad-dimers on the surface: Many body potential calculations," *Phys. Rev. B* **64**, 035402 (2001).
67. J.-S. Wang and R. H. Swendsen, "Transition matrix Monte Carlo method," *J. Stat. Phys.* **106**, 245 (2002).
68. J.-S. Wang, "Flat-histogram and free energy calculation," in 'OCPA 2000: Proceedings of the Third Joint Meeting of Chinese Physicists Worldwide', p.244, N.-P. Chang, K. Young, H. M. Lai, C.-Y. Wong (eds.), World Scientific, Singapore (2002).
69. J.-S. Wang, "Efficient Monte Carlo simulation methods in statistical physics," in 'Monte Carlo and Quasi-Monte Carlo Methods 2000', p.141, K.-T. Fang, F. J. Hickernell, and H. Niederreiter (eds.), Springer-Verlag, Berlin (2002).
70. J. Cai and J.-S. Wang, "Reconstruction of Si(001): a comparison study of many body potential calculations," *Phys. Stat. Sol. (b)* **223**, 773 (2001).
71. J. Cai and J.-S. Wang, "Molecular dynamics study of the friction properties for a Ge tip-surface system," in 'Proceedings of the International Symposium on the Science of Surface and Nanostructures', *Surface Review Letters*, **8**, 581 (2001).
72. L. Yi and J.-S. Wang, "Universal quantum fluctuations and crossover phenomena in tunneling through small Coulomb islands," *Chin. Phys. Lett.* **19**, 1333 (2002).
73. L. Yi and J.-S. Wang, "Interference effects, universal fluctuations, and crossing phenomena in the intermediate coupling regime: strongly interacting transport," *Phys. Rev. B* **66**, 085105 (2002).
74. L. Yi and J.-S. Wang, "Interference and coherence in electron tunnelings through quantum dots," *Phys. Lett. A* **301**, 327 (2002).
75. J.-S. Wang, "Methods for computing density of states for statistical mechanical models," in *Computer Simulation Studies in Condensed Matter Physics XIV*, p. 113, Eds. D. P. Landau, S. P. Lewis, and H. B. Schuettler (Springer Verlag, Heidelberg, 2002).
76. J. Cai and J.-S. Wang, "Friction between a Ge tip and the (001)-2×1 surface: A molecular-dynamics simulation," *Phys. Rev. B* **64**, 113313 (2001).
77. D. Chowdhury and J.-S. Wang, "Flow properties of driven-diffusive lattice gases: theory and computer simulation," *Phys. Rev. E* **65**, 046126 (2002).
78. L. W. Lee and J.-S. Wang, "Flat histogram simulation of lattice polymer systems," *Phys. Rev. E* **64**, 056112 (2001).
79. X. S. Gao, J. Lim, J. M. Xue, J.-S. Wang, and J.-M. Liu, and J. Wang, "A Monte-Carlo simulation of B site order-disorder transformation in Pb[Sc(1/2)Ta(1/2)]O₃ triggered by mechanical activation," *J. Phys. condensed-matter*, **14**, 8639 (2002).
80. J.-S. Wang, O. Kozan, and R. H. Swendsen, "Binary tree summation Monte Carlo method for Potts models," in *Computer Simulation Studies in Condensed Matter Physics XV*, p.189, Eds. D. P. Landau, S. P. Lewis, and H. B. Schuettler (Springer Verlag, Heidelberg, 2002).
81. J. Cai and J.-S. Wang, "Adsorption and diffusion of Si on the Si(001): an empirical potential calculation," *Inter. J. Mod. Phys. B* **16**, 621 (2002).
82. J.-S. Wang, O. Kozan, R. H. Swendsen, "Sweeny and Gliozzi dynamics for simulations of Potts models in the Fortuin-Kasteleyn representation," *Phys. Rev. E* **66**, 057101 (2002).
83. J.-S. Wang, "Binary tree summation Monte Carlo simulation for Potts models," in *Statphys-Taiwan 2002 conference proceedings*, *Physica A* **321**, 351 (2003).
84. J. Cai and J.-S. Wang, "Modeling generalized stacking fault in Au using tight-binding potential combined with a simulated annealing method," *Euro. Phys. J. B* **28**, 45 (2002).
85. J. Cai and J.-S. Wang, "Energies and structure of stacking faults of Ag from the tight-binding method calculation," *Modeling Simul. Mater. Sci. Eng.* **10**, 469 (2002).

86. J. Cai and J.-S. Wang, “Friction between Si tip and (001)-2×1 surface: A molecular-dynamics simulation,” *Comp. Phys. Comm.* **147**, 145 (2002).
87. J.-S. Wang and Y. Okabe, “A comparison of extremal optimization with flat-histogram dynamics for finding spin-glass ground states,” *J. Phys. Soc. Jpn.* **72**, 1380 (2003).
88. A. D. Güçlü, J.-S. Wang, H. Guo, “Disordered quantum dots: a diffusion quantum Monte Carlo study,” *Phys. Rev. B* **68**, 035304 (2003).
89. J.-S. Wang, “Transition matrix Monte Carlo and flat-histogram algorithm,” in AIP conference proceedings 690: ‘The Monte Carlo Method in the Physical Sciences, Celebrating the 50th Anniversary of the Metropolis Algorithm, Los Alamos, 2003’. ed. J. E. Gubernatis, p.344.
90. J.-S. Wang and B. Li, “Intriguing heat conduction of a chain with transverse motions,” *Phys. Rev. Lett.* **92**, 074302 (2004).
91. H. A. Wu, G. R. Liu and J.-S. Wang, “Atomistic and continuum simulation on extension behaviour of single crystal with nano holes,” *Modelling Simul. Mater. Sci. Eng.*, **12**, 225 (2004).
92. J.-S. Wang and B. Li, “Mode-coupling theory and molecular dynamics simulation for heat conduction in a chain with transverse motions,” *Phys. Rev. E* **70**, 021204 (2004).
93. Z. Yao and J.-S. Wang, G. Liu, and M. Cheng “Improved neighbor list algorithm by using cell decomposition and data sorting method,” *Comput. Phys. Comm.* **161**, 27 (2004).
94. Z. Yao, J.-S. Wang, B. Li, G.-R. Liu, “Thermal conduction of Carbon nanotubes using molecular dynamics,” *Phys. Rev. B* **71**, 085417 (2005).
95. J.-S. Wang and R. H. Swendsen, “Replica Monte Carlo simulation (revisited),” *Prog. Theor. Phys. Supp.* **157**, 317 (2005).
96. Y.-Q. Zhang, G.-R. Liu, J.-S. Wang, “Small scale effects on buckling of multi-walled carbon nanotubes under axial compression,” *Phys. Rev. B* **70**, 205430 (2004).
97. J.-S. Wang, “Worm algorithm for two-dimensional spin glasses,” *Phys. Rev. E* **72**, 036706 (2005).
98. R. Sugiarto, L. Han, J.-S. Wang, and Y. Z. Chen, “Super paramagnetic clustering of DNA sequences,” *J. Biological Phys.* **32**, 11 (2006).
99. D. Mi, G.-R. Liu, J.-S. Wang, and Z. R. Li, “Relationships between the folding rate constant and the topological parameters of small two-state proteins based on general random walk model,” *J. theo. Bio.* **241**, 152 (2006).
100. J. Wang and J.-S. Wang, “Mode-dependent energy transmission across nanotube junctions calculated with a lattice dynamics approach,” *Phys. Rev. B* **74**, 054303 (2006).
101. J. Wang and J.-S. Wang, “Carbon nanotube thermal transport: ballistic and diffusive,” *Appl. Phys. Lett.* **88**, 111909 (2006).
102. J. Du, B. Zheng, and J.-S. Wang, “Dynamic critical exponents for Swendsen-Wang and Wolff algorithms obtained by a nonequilibrium relaxation method,” *J. Stat. Mech.: theo. exp.* P05004 (2006).
103. J.-S. Wang, J. Wang, and N. Zeng, “Nonequilibrium Green’s function approach to mesoscopic thermal transport,” *Phys. Rev. B* **74**, 033408 (2006).
104. J. Wang and J.-S. Wang, “Characteristics of phonon transmission across epitaxial interfaces: a lattice dynamic study,” *J. Phys.: Condens. Matter*, **19**, 236211 (2007).
105. D. Duong-Hong, J.-S. Wang, G.-R. Liu, Y. Z. Chen, J. Han, and N. G. Hadjiconstantinou, “Dissipative particle dynamics simulations of electroosmotic flow in nano-fluidic devices,” *Microfluidics and Nanofluidics*, **4**, 219 (2008).
106. J.-S. Wang, N. Zeng, J. Wang, and C. K. Gan, “Nonequilibrium Green’s function method for thermal transport in junctions,” *Phys. Rev. E* **75**, 061128 (2007).
107. J. T. Lü and J.-S. Wang, “Coupled electron and phonon transport in one-dimensional atomic junctions,” *Phys. Rev. B* **76**, 165418 (2007).

108. J. Wang and J.-S. Wang, “Dimensional crossover of thermal conductance in nanowires,” *Appl. Phys. Lett.* **90**, 241908 (2007).
109. J.-S. Wang, “Quantum thermal transport from classical molecular dynamics,” *Phys. Rev. Lett.* **99**, 160601 (2007).
110. Z. Li, G. R. Liu, Y. Z. Chen, J.-S. Wang, H. Bow, Y. Cheng, and J. Han, “Continuum transport model of Ogston sieving in patterned nanofilter arrays for separation of rod-like biomolecule separation,” *Electrophoresis*, **29**, 329 (2008).
111. D. Chowdhury and J.-S. Wang, “Traffic of single-headed motor proteins KIF1A: effects of lane changing,” *Phys. Rev. E* **77**, 050902(R) (2008).
112. J.-S. Wang, J. Wang, and J. T. Lü, “Quantum thermal transport in nanostructures,” *Eur. Phys. J. B*, **62**, 381 (2008).
113. J. T. Lü and J.-S. Wang, “Coupled electron-phonon transport from molecular dynamics with quantum baths,” *J. Phys.: Condens. Matter*, **21**, 025503 (2009).
114. N. Zeng and J.-S. Wang, “Mechanisms causing thermal rectification: the influence of phonon frequency, asymmetry, and nonlinear interactions,” *Phys. Rev. B* **78**, 024305 (2008).
115. D. Chowdhury, A. Garai, P. Greulich, K. Nishinari, A. Schadschneider, T. Tripathi, and J.-S. Wang, “From CA to gene expression: machines and mechanisms,” in *Lecture Notes in Computer Science*, vol 5191, 1 (2008).
116. N. Zeng and J.-S. Wang, “Thermal rectification in one-dimensional chain,” in ‘Recent Progress in Many-Body Theories: Proceedings of the 14th International Conference, Barcelona,’ p.431, J Boronat, G. E. Astrakharchik, and F. Mazzanti, eds. (World Scientific, 2008).
117. R. Wang, J.-S. Wang, G.-R. Liu, J. Han, and Y.-Z. Chen, “Simulation of DNA electrophoresis in systems of large number of solvent particles by coarse-grained hybrid molecular dynamics approach,” *J. Comput. Chem.* **30**, 505 (2008).
118. M. Hu, P. Keblinski, J.-S. Wang, and N. Ravivakar, “Interfacial thermal conductance between silicon and a vertical carbon nanotube,” *J. Appl. Phys.* **104**, 083503 (2008).
119. Y. Xu, J.-S. Wang, B. Li, J. Wu, B.-L. Gu, and W. Duan, “Nonequilibrium Green’s function method for phonon-phonon interaction and ballistic-diffusive thermal transport,” *Phys. Rev. B*, **78**, 224303 (2008).
120. J. T. Lü and J.-S. Wang, “Quantum phonon transport of molecular junctions amide-linked with carbon nanotubes: a first-principles study,” *Phys. Rev. B* **78**, 235436 (2008).
121. J. Wang and J.-S. Wang, “Single-mode phonon transmission in symmetry broken carbon nanotubes: role of phonon symmetries,” *J. Appl. Phys.* **105**, 063509 (2009).
122. L. Zhang, J.-S. Wang, and B. Li, “Ballistic magneto-thermal transport in a Heisenberg spin chain at low temperatures,” *Phys. Rev. B* **78**, 144416 (2008).
123. J. Lan, J.-S. Wang, C. K. Gan, and S. K. Chin, “Edge effects of quantum thermal transport in graphene ribbons: tight-binding calculations,” *Phys. Rev. B* **79**, 115401 (2009).
124. Z. R. Li, G. R. Liu, J. Han, Y. Cheng, Y. Z. Chen, J.-S. Wang, and N. G. Hadjiconstantinou, “Analytical description of Ogston-regime biomolecule separation using nanofilters and nanopores,” *Phys. Rev. E*, **80**, 041911 (2009).
125. Z. R. Li, G. R. Liu, J. Han, Y. Z. Chen, J.-S. Wang, and N. Hadjiconstantinou, “Transport of biomolecules in asymmetric nanofilter arrays,” *Anal. Bioanal. Chem.* **394**, 427 (2009).
126. X. Gao, J.-S. Wang, G.-R. Liu, Y. Z. Chen, J. Han, D.-H. Duc, “Establishing structure-function relationship for molecular sieving: dissipative particle dynamics simulations of DNA polymers,” in preparation.
127. E. Cuansing and J.-S. Wang, “Quantum transport in honeycomb lattice ribbons with armchair and zigzag edges coupled to semi-infinite linear chain leads,” *Eur. Phys. J. B* **69**, 505 (2009).

128. Y.-Z. Sun, L. Yi, and J.-S. Wang, “Effects of Dzyaloshinsky-Moriya interaction on planar rotator model on triangular lattice,” *Commun. Comput. Phys.* **11**, 1169 (2012).
129. J.-S. Wang and L. Zhang, “Phonon Hall thermal conductivity from Green-Kubo formula,” *Phys. Rev. B* **80**, 012301 (2009).
130. L. Zhang, J.-S. Wang, and B. Li, “Phonon Hall effect in four-terminal junctions,” *New J. Phys.* **11**, 113038 (2009).
131. J.-W. Jiang, J.-S. Wang, and B. Li, “Thermal conductance of graphene and dimerite,” *Phys. Rev. B* **79**, 205418 (2009).
132. J.-W. Jiang, J. Chen, J.-S. Wang, and B. Li, “Edge states induce boundary temperature jump in molecular dynamics simulation of heat conduction,” *Phys. Rev. B* **80**, 052301 (2009).
133. J.-S. Wang, X. Ni, and J.-W. Jiang, “Molecular dynamics with quantum heat baths: results for nanoribbons and nanotubes,” *Phys. Rev. B* **80**, 224302 (2009).
134. G. Liang, W. Huang, C. S. Koong, J.-S. Wang, and J. Lan, “Geometry effects on thermoelectric properties of silicon nanowires based on electronic band structures,” *J. Appl. Phys.* **107**, 014317 (2010).
135. J.-W. Jiang, J.-S. Wang, and B. Li, “Young’s modulus of graphene: A molecular dynamics study,” *Phys. Rev. B* **80**, 113405 (2009).
136. J.-W. Jiang, J.-S. Wang, and B. Li, “Topology-induced thermal rectification in carbon nanodevice,” *Europhys. Lett.* **89**, 46005 (2010).
137. X. Ni, G. Liang, J.-S. Wang, and B. Li, “Disorder enhances thermoelectric figure of merit in armchair graphene nanoribbons,” *Appl. Phys. Lett.* **95**, 192114 (2009).
138. J.-W. Jiang, J.-S. Wang, and B. Li, “Thermal expansion in carbon nanotubes and graphene: nonequilibrium Green’s function approach,” *Phys. Rev. B* **80**, 205429 (2009).
139. L. Zhang, Y. Yan, C.-Q. Wu, J.-S. Wang, B. Li, “Reversal of thermal rectification in quantum systems,” *Phys. Rev. B* **80**, 172301 (2009).
140. E. C. Cuansing and J.-S. Wang, “Transient behavior of heat transport in a thermal switch,” *Phys. Rev. B* **81**, 052302 (2010).
141. J.-W. Jiang, J.-S. Wang, and B. Li, “Thermal contraction in silicon nanowires at low temperatures,” *Nanoscale*, **2**, 2864 (2010).
142. Hu, L. Zhang, M. Hu, J.-S. Wang, B. Li, and P. Keblinski, “Phonon interference at self-assembled monolayer interfaces: Molecular dynamics simulations,” *Phys. Rev. B* **81**, 235427 (2010).
143. L. Zhang, J.-S. Wang, and B. Li, “Ballistic thermal rectification in nanoscale three-terminal junctions,” *Phys. Rev. B* **81**, 100301(R) (2010).
144. Y. Xu, X. Chen, J.-S. Wang, B.-L. Gu, and W. Duan, “Thermal transport in graphene junctions and quantum dots,” *Phys. Rev. B* **81**, 195425 (2010).
145. Z. R. Li, G. R. Liu, N. G. Hadjiconstantinou, J. Han, J.-S. Wang, and Y. Z. Chen, “Dispersive transport of biomolecules in periodic energy landscapes with application to nanofilter sieving arrays,” *Electrophoresis*, **32**, 506 (2011).
146. J.-W. Jiang, J.-S. Wang, and B. Li, “Elastic and nonlinear stiffness of graphene: A simple approach,” *Phys. Rev. B* **81**, 073405 (2010).
147. J.-W. Jiang, J. Lan, J.-S. Wang, and B. Li, “Isotopic effects on the thermal conductivity of graphene nanoribbons: localization mechanism,” *J. Appl. Phys.* **107**, 054314 (2010).
148. X. Ni, M. L. Leek, J.-S. Wang, Y. P. Feng, and B. Li, “Anomalous thermal transport in disordered harmonic chains and carbon nanotubes,” *Phys. Rev. B* **83**, 045408 (2011).
149. J.-W. Jiang and J.-S. Wang, “Conditions for the existence of phonon localized edge-modes,” *Phys. Rev. B* **81**, 174117 (2010).

150. E. C. Cuansing and J.-S. Wang, "A tunable heat pump by modulating the coupling to the leads," *Phys. Rev. E* **82**, 021116 (2010).
151. Z. B. Siu, M. B. A. Jalil, S. G. Tan, and J.-S. Wang, "A self-consistent SDD-NEGF approach for modelling magnetic tunnel junctions," *IEEE Transactions on Magnetics* **46**, 1591 (2010).
152. J.-W. Jiang and J.-S. Wang, "Self-repairing in single-walled carbon nanotubes by heat treatment," *J. Appl. Phys.* **108**, 054303 (2010).
153. B. K. Agarwalla, L. Zhang, J.-S. Wang, and B. Li, "Phonon Hall effect in ionic crystals in the presence of static magnetic field," *Eur. Phys. J. B* **81**, 197 (2011).
154. L. Zhang, J. Ren, J.-S. Wang, and B. Li, "Topological nature of phonon Hall effect," *Phys. Rev. Lett.* **105**, 225901 (2010).
155. Z. W. Tan, J.-S. Wang, and C. K. Gan, "First-principles study of heat transport properties of graphene nanoribbons," *Nano Lett.* **11**, 214 (2011).
156. J.-W. Jiang, J.-S. Wang, and B. Li, "Topological effect on thermal conductivity in graphene," *J. Appl. Phys.* **108**, 064307 (2010).
157. J.-W. Jiang and J.-S. Wang, "A universal exponential factor in the dimensional crossover from graphene to graphite," *J. Appl. Phys.* **108**, 124311 (2010).
158. J.-W. Jiang, B.-S. Wang, J.-S. Wang, "First principle study of the thermal conductance in graphene nanoribbon with vacancy and substitutional silicon defects," *Appl. Phys. Lett.* **98**, 113114 (2011).
159. J.-W. Jiang, J.-S. Wang, B. Li, "A nonequilibrium Green's function study of thermoelectric properties in single-walled carbon nanotubes," *J. Appl. Phys.* **109**, 014326 (2011).
160. W. Huang, J.-S. Wang, G. Liang, "Theoretical study on thermoelectric properties of kinked graphene nanoribbons," *Phys. Rev. B* **84**, 045410 (2011).
161. J. Thingna and J.-S. Wang, "Geometric effects on spin injection: 3D spin drift diffusion model," *J. Appl. Phys.* **109**, 124303 (2011).
162. L. Zhang, P. Keblinski, J.-S. Wang, and B. Li, "Interfacial thermal transport in atomic junctions," *Phys. Rev. B* **83**, 064303 (2011).
163. L. Zhang, J. Ren, J.-S. Wang, and B. Li, "The phonon Hall effect: theory and application," *J. Phys.: Condens. Matter* **23**, 305402 (2011).
164. J.-W. Jiang and J.-S. Wang, "Theoretical study of thermal conductivity in single-walled boron nitride nanotubes," *Phys. Rev. B* **84**, 085439 (2011).
165. J.-W. Jiang, B.-S. Wang, and J.-S. Wang, "Minimum thermal conductance in graphene and boron nitride superlattice," *Appl. Phys. Lett.* **99**, 043109 (2011).
166. B. K. Agarwalla, J.-S. Wang, and B. Li, "Heat generation and transport due to time-dependent forces," *Phys. Rev. E*, **84**, 041115 (2011).
167. J.-W. Jiang, B.-S. Wang, and J.-S. Wang, "Molecular dynamics simulation for heat transport in thin diamond nanowires," *Phys. Rev. B* **83**, 235432 (2011).
168. J.-W. Jiang and J.-S. Wang, "Manipulation of heat current by the interface between graphene and white graphene," *Europhys. Lett.* **96**, 16003 (2011).
169. E. C. Cuansing, H. Li, and J.-S. Wang, "Role of the on-site pinning potential in establishing quasi-steady-state conditions in heat transport in finite quantum systems," *Phys. Rev. E* **86**, 031132 (2012).
170. J.-S. Wang, B. K. Agarwalla, and H. Li, "Transient behavior of full counting statistics in thermal transport," *Phys. Rev. B* **84**, 153412 (2011).
171. J.-W. Jiang and J.-S. Wang, "Graphene-based torsional resonator from molecular dynamics simulation," *Europhys. Lett.* **96**, 66007 (2011).

172. J. Wang, L. Li, and J.-S. Wang, "Tuning thermal transport in nanotubes with topological defects," *Appl. Phys. Lett.* **99**, 091905 (2011).
173. J.-W. Jiang and J.-S. Wang, "Joule heating and thermoelectric properties in short single-walled carbon nanotubes: electron-phonon interaction effect," *J. Appl. Phys.* **110**, 124319 (2011).
174. J.-W. Jiang and J.-S. Wang, "Bright and dark modes induced by graphene bubbles," *Europhys. Lett.* **97**, 36004 (2012).
175. B. K. Agarwalla, B. Li, and J.-S. Wang, "Full-counting statistics of heat transport in harmonic junctions: transient, steady states, and fluctuation theorems," *Phys. Rev. E* **85**, 051142 (2012).
176. J.-W. Jiang and J.-S. Wang, "Why edge effects are important on the intrinsic loss mechanisms of graphene nanoresonators?" *J. Appl. Phys.* **111**, 054314 (2012).
177. K. Yan, Y.-Z. Chen, J. Han, G.-R. Liu, J.-S. Wang, and N. G. Hadjiconstantinou, "Dissipative particle dynamics simulation of field-dependent DNA mobility in nanoslits," *Microfluidics and Nanofluidics*, **12**, 157 (2012).
178. X. Lu, J.-S. Wang, W. G. Morrel, X. Ni, C.-Q. Wu, and B. Li, "Thermoelectric effect in Aharonov-Bohm structures," *J. Phys.: Condens. Matter*, **27**, 035301 (2015).
179. J. Thingna, J. L. García-Palacios, and J.-S. Wang, "Steady-state thermal transport in anharmonic systems: application to molecular junctions," *Phys. Rev. B* **85**, 195452 (2012).
180. J. Wang, X.-M. Wang, Y.-F. Chen, and J.-S. Wang, "Dimensional crossover of thermal conductance in graphene nanoribbons: a first-principles approach," *J. Phys.: Condens. Matter* **24**, 295403 (2012).
181. J. Thingna, J.-S. Wang, and P. Hänggi, "Generalized Gibbs state with modified Redfield solution: Exact agreement up to second order," *J. Chem. Phys.* **136**, 194110 (2012).
182. L. Zhang, J. Ren, J.-S. Wang, and B. Li, "Topological magnon insulator in insulating ferromagnet," *Phys. Rev. B* **87**, 144101 (2013).
183. L. Zhang, J.-T. Lü, J.-S. Wang, and B. Li, "Thermal transport across metal-insulator interface via electron-phonon interactions," *J. Phys.: Condens. Matter* **25**, 445801 (2013).
184. H. Li, B. K. Agarwalla, and J.-S. Wang, "Generalized Caroli formula for transmission coefficient with lead-lead coupling," *Phys. Rev. E* **86**, 011141 (2012).
185. H. Li, B. K. Agarwalla, and J.-S. Wang, "Cumulant generating function formula of heat transfer in ballistic systems with lead-lead coupling," *Phys. Rev. B* **86**, 165425 (2012).
186. H. Li, B. K. Agarwalla, B. Li, and J.-S. Wang, "Cumulants of heat transfer in nonlinear quantum systems," *Eur. Phys. J. B*, **86**, 500 (2013).
187. S. Liu, B. K. Agarwalla, J.-S. Wang, and B. Li, "Classical heat transport in anharmonic molecular junctions: exact solutions," *Phys. Rev. E* **87**, 022122 (2013).
188. Z. Q. Bai, L. Shen, Q. Y. Wu, M. G. Zeng, J.-S. Wang, G. Han, and Y. P. Feng, "Boron diffusion induced symmetry reduction and scattering in CoFeB/MgO/CoFeB magnetic tunnel junctions," *Phys. Rev. B* **87**, 014114 (2013).
189. L. Zhang, J. Thingna, D. He, J.-S. Wang, and B. Li, "Nonlinearity enhanced interfacial thermal conductance and rectification," *EPL*, **103**, 64002 (2013).
190. J.-S. Wang, B. K. Agarwalla, H. Li, and J. Thingna, "Nonequilibrium Green's function method for quantum thermal transport," *Front. Phys.* **9**, 673 (2014).
191. J. Thingna, J.-S. Wang, and P. Hänggi, "Reduced density matrix for nonequilibrium steady states: A modified Redfield solution approach," *Phys. Rev. E* **88**, 052127 (2013).
192. J. Thingna and J.-S. Wang, "Spin rectification in thermally driven XXZ spin chain via spin-Seebeck effect," *EPL*, **104**, 37006 (2013).
193. K. Rubi, P. Kumar, D. V. M. Repaka, R. Chen, J.-S. Wang, and R. Mahendiran, "Giant magnetocaloric effect in magnetoelectric $\text{Eu}_{1-x}\text{Ba}_x\text{TiO}_3$," *Applied Phys. Lett.* **104**, 032407 (2014).

194. J. Lan, Y. Cai, G. Zhang, J.-S. Wang, and Y.-W. Zhang, “Topological symmetry-induced width dependence of thermal conductance of edge-reconstructed graphene nanoribbons,” *J. Phys. D: Appl. Phys.* **47** 265303 (2014).
195. J.-W. Jiang, B.-S. Wang, J.-S. Wang, and H. S. Park, “A review on flexural mode of graphene: lattice dynamics, thermal conduction, thermal expansion, elasticity, and nanomechanical resonance,” *J. Phys.: Condens. Matter*, **27**, 083001 (2015).
196. J. Thingna, H. Zhou, and J.-S. Wang, “Improved Dyson series expansion for steady-state quantum transport beyond the weak coupling limit - divergences and resolution,” *J. Chem. Phys.* **141**, 194101 (2014).
197. H. Zhou, J. Thingna, J.-S. Wang, and B. Li, “Thermoelectric transport through a quantum nano-electromechanical system and its backaction,” *Phys. Rev. B* **91**, 045410 (2015).
198. J.-T. Lü, R. B. Christensen, J.-S. Wang, P. Hedegård, and M. Brandbyge, “Current-induced forces and hot-spots in biased nano-junctions,” *Phys. Rev. Lett.* **114**, 096801 (2015).
199. H. Zhou, J. Thingna, P. Hänggi, J.-S. Wang, and B. Li, “Boosting thermoelectric efficiency using time-dependent control,” *Sci. Rep.* **5**, 14870 (2015).
200. R. H. Swendsen and J.-S. Wang, “Gibbs volume entropy is incorrect,” *Phys. Rev. E* **92**, 020103(R) (2015).
201. R. H. Swendsen and J.-S. Wang, “Negative temperatures and the definition of entropy,” *Physica A* **453**, 24 (2016).
202. J.-S. Wang, “Critique on Gibbs volume entropy and its implication,” unpublished
203. J.-T. Lü, H. Zhou, J.-W. Jiang, and J.-S. Wang, “Effects of electron-phonon interaction on thermal and electrical transport through molecular nano-conductors,” *AIP Advances*, **5**, 053204 (2015).
204. A. Midya, P. Mandal, K. Rubi, R. Chen, J.-S. Wang, R. Mahendiran, G. Lorusso, and M. Evangelisti, “Large adiabatic temperature and magnetic entropy changes in EuTiO_3 ,” *Phys. Rev. B* **93**, 094422 (2016).
205. J.-T. Lü, J.-S. Wang, P. Hedegård, and M. Brandbyge, “Electron and phonon drag in thermoelectric transport through coherent molecular conductors,” *Phys. Rev. B* **93**, 205404 (2016).
206. D. He, J. Thingna, J.-S. Wang, and B. Li, “Quantum thermal transport through anharmonic systems: a self-consistent approach,” *Phys. Rev. B* **94**, 155411 (2016).
207. J.-P. Lv and J.-S. Wang, “Bosonic Haldane insulator in the presence of local disorder: A quantum Monte Carlo study,” *EPL*, **123**, 10004 (2018).
208. J.-S. Wang and J. Peng, “Capacitor physics in ultra-near-field heat transfer,” *EPL* **118**, 24001 (2017).
209. H. Zhou, G. Zhang, J.-S. Wang, and Y.-W. Zhang, “Phonon transport in a one-dimensional harmonic chain with long-range interaction and mass disorder,” *Phys. Rev. E* **94**, 052123 (2016).
210. H. H. Yap and J.-S. Wang, “Radiative heat transfer as a Landauer-Büttiker problem,” *Phys. Rev. E* **95**, 012126 (2017).
211. X. Xu, J. Thingna, and J.-S. Wang, “Finite coupling effects in double quantum dots near equilibrium,” *Phys. Rev. B* **95**, 035428 (2017).
212. R. Chen, J.-C. Ren, K. Rubi, R. Mahendiran, and J.-S. Wang, “Strong electron-phonon interaction and colossal magnetoresistance in EuTiO_3 ,” *Euro. Phys. J. B*, **91**, 36 (2018).
213. J.-H. Jiang and J.-S. Wang, “Caroli formalism in near field heat transfer between parallel graphene sheets,” *Phys. Rev. B* **96**, 155437 (2017).
214. H. H. Yap, L. Zhou, J.-S. Wang, and J. Gong, “Computational study of the two-terminal transport of Floquet quantum Hall insulators,” *Phys. Rev. B* **96**, 165443 (2017).

215. K. Yang, J. Ren, H. Qiu, and J.-S. Wang, "Phonon-driven electron scattering and magnetothermoelectric effect in two-dimensional tin selenide," *J. Phys.: Condens. Matter* **30**, 055301 (2018).
216. S. Li, T.-Y. Lue, J.-C. Zheng, S.-W. Yang, J.-S. Wang, and G. Wu, "Origin of metallicity in 2D multilayer Mickle Bis(ditheiolene) Sheets," *2D Materials* **5**, 035027 (2018).
217. E. Yildirim, G. Wu, Y. Xue, T.L. Tan, Z. Qiang, J. Xu, J. Ouyang, J.-S. Wang, S. W. Yang, "A theoretical mechanistic study on electrical conductivity enhancement of DMSO treated PEDOT:PSS," *J. Materials Chemistry C* **6**, 5122 (2018).
218. Z.-Q. Zhang, J.-T. Lü, and J.-S. Wang, "Energy transfer between two vacuum-gapped metal plates: Coulomb fluctuations and electron tunneling," *Phys. Rev. B* **97**, 195450 (2018).
219. J.-S. Wang, Z.-Q. Zhang, and J.-T. Lü, "Coulomb-force-mediated heat transfer in the near field: geometric effect," *Phys. Rev. E* **98**, 012118 (2018).
220. W. Shi, G. Wu, X. Yong, T. Deng, J.-S. Wang, J.-C. Zheng, J. Xu, M. B. Sullivan, and S.-W. Yang, "Orbital-engineering based screening of pi-conjugated d8 transition-metal coordination polymers for high-performance n-type thermoelectric applications," *ACS Appl. Mater. Interfaces*, **10**, 35306 (2018).
221. G. Tang and J.-S. Wang, "Heat transfer statistics in extreme-near field radiation," *Phys. Rev. B* **98**, 125401 (2018).
222. X. Yong, W. Shi, G. Wu, S. S. Goh, S. Bai, J. Xu, J.-S. Wang, and S.-W. Yang, "Tuning thermoelectric performance of -d conjugated nickel coordination polymers through metalligand frontier molecular orbital alignment," *J. Mater. Chem. A*, **6**, 19757 (2018).
223. E. C. Cuansing and J.-S. Wang, "Quantum engine by pumping electrons in a nanojunction with a single gate and dynamic tunnel couplings to the leads," *Proceedings of the Samahang Pisika ng Pilipinas* **36**, SPP-2018-3B-01 (2018).
224. W. Shi, G. Wu, K. Hippalgaonkar, J.-S. Wang, J. Xu, S.-W. Yang, "Poly(nickel-ethylenetetra-thiolate) and its analogs: Theoretical prediction of high-performance doping-free thermoelectric polymers," *J. Am. Chem. Soc.* **140**, 13200 (2018).
225. G. Tang, J. Peng, and J.-S. Wang, "Three-terminal normal-superconductor junction as thermal transistor," *Eur. Phys. J. B* **92**, 27 (2019).
226. G. Tang, H. H. Yap, J. Ren, and J.-S. Wang, "Anomalous near-field heat transfer in carbon-based nanostructures with edge states," *Phys. Rev. Appl.* **11**, 031004 (2019).
227. T. Deng, X. Yong, W. Shi, C.-. Gan, W. Li, K. Hippalgaonkar, J.-C. Zheng, X. Wang, S.-W. Yang, J.-S. Wang, and G. Wu, "2D single-layer pi-conjugated nickel bis(dithiolene) complex: a good-electron-poor-phonon thermoelectric material," *Advanced Electronic Materials*, 1800892 (2019).
228. G. Xiong, Z. Yu, J.-S. Wang, and L. Zhang, "Phonon quarters-wave loss," *New J. Phys.* **21**, 093046 (2019).
229. G. Xiong, J.-S. Wang, D. Ma, L. Zhang, "Dramatic enhancement of interfacial thermal transport by mass-graded and coupling-graded materials," *EPL*, **128**, 54007 (2020).
230. Z. Gao, M. Li and J.-S. Wang, "Insight into two-dimensional borophene: five-center bond and phonon-mediated superconductivity," *ACS Applied Materials & Interfaces*, **11**, 47279 (2019).
231. Z. Gao, Z. Zhang, G. Liu, and J.-S. Wang, "Ultra-low lattice thermal conductivity of monolayer penta-silicene and penta-germanene," *Phys. Chem. Chem. Phys.* **21**, 26033 (2019).
232. Z. Gao and J.-S. Wang, "Thermoelectric penta-silicene with a high room-temperature figure of merit," *ACS Applied Materials & Interfaces*, **12**, 14298 (2020).
233. T. Deng, X. Yong, W. Shi, Z. M. Wong, G. Wu, H. Pan, J.-S. Wang, S.-W. Yang, "Beyond Mahan-Sofo best thermoelectric: high thermoelectric performance from directional -conjugation in two-dimensional poly(tetrathienoanthracene)," *J. Mater. Chem. A*, **8**, 4257 (2020).

- 234.** G. Wu, T. Deng, M. Sullivan, Z. Wong, K. Hippalgaonkar, J.-S. Wang, and S.-W. Yang, “EPIC STAR: a reliable and efficient approach for phonon- and impurity-limited charge transport calculations,” *npj Computational Materials*, **6**, 46 (2020).
- 235.** K. N. Lian and J.-S. Wang, “Geometric effect on near-field heat transfer analysis using efficient graphene and nanotube models,” *Eur. Phys. J. B* **93**, 138 (2020).
- 236.** T. Zhu, Z.-Q. Zhang, Z. Gao, and J.-S. Wang, “First-principles method to study near-field radiative heat transfer”, *Phys. Rev. Applied* **14**, 024080 (2020).
- 237.** X. Liu, Z. Zhang, Z. Ding, B. Lv, Z. Luo, J.-S. wang, and Z. Gao, “Highly anisotropic electronic and mechanical properties of monolayer and bilayer As₂S₃,” *Applied Surface Science* **542**, 148665 (2021).
- 238.** K. Sun, Z. Gao, and J.-S. Wang, “Current-induced phonon Hall effect,” *Phys. Rev. B* **102**, 134311 (2020).
- 239.** Y.-M. Zhang and J.-S. Wang, “Far-field heat and angular momentum radiation of the Haldane model,” *J. Phys.:Condens. Matter* **33**, 055301 (2021).
- 240.** X. Yong, G. Wu, W. Shi, Z. M. Wong, T. Deng, Q. Zhu, X. Yang, J.-S. Wang, J. Xu, and S.-W. Yang, “Theoretical search for high-performance thermoelectric donor-acceptor copolymers: the role of super-exchange couplings,” *J. Mater. Chem. A* **8**, 21852 (2020).
- 241.** L.-L. Nian, T. Wang, Z.-Q. Zhang, J.-S. Wang, and J.-T. L, “Effective Control of photon statistics from electroluminescence by a Fano-like interference effect,” *J. Phys. Chem. Lett.***11**, 8721 (2020).
- 242.** K. Wang, X. Xu, Y. Cheng, M. Zhang, J.-S. Wang, H. Wang, and G. Zhang, “Magnon-magnon interaction and magnon relaxation time in a ferromagnetic Cr₂Ge₂Te₆ monolayer,” *Phys. Rev. B* **102**, 235434 (2020).
- 243.** K. Wang, X. Xu, Y. Cheng, M. Zhang, J.-S. Wang, H. Wang, and G. Zhang, “Magnon relaxation time in ferromagnetic Cr₂Ge₂Te₆ monolayer governed by magnon-phonon interaction,” *Appl. Phys. Lett.* **118**, 023102 (2021).
- 244.** J.-S. Wang, “Phonon soft modes and para- to ferro-electric phase transitions,” *Physica A* **566**, 125641 (2021).
- 245.** T. Deng, G. Wu, W. Shi, Z. M. Wong, J.-S. Wang, S.-W. Yang, “Ab initio dipolar electron-phonon interactions in two-dimensional materials,” *Phys. Rev. B* **103**, 075410 (2021).
- 246.** T. Zhu, M. Antezza, J.-S. Wang, “Dynamical polarizability of graphene with spatial dispersion,” *Phys. Rev. B* **103**, 125421 (2021).
- 247.** K. Sun, Z. Gao, and J.-S. Wang, “Phonon Hall effect with first-principles calculations,” *Phys. Rev. B* **103**, 214301 (2021).
- 248.** R. Zhu, Z. Gao, Q. Liang, J. Hu, J.-S. Wang, C.-W. Qiu, and A.T.S. Wee, “Observation of anisotropic magnetoresistance in layered nonmagnetic semiconducting PdSe₂,” *ACS Applied Materials & interfaces*, **13**, 37527 (2021).
- 249.** T. Zhu and J.-S. Wang, “Generalized first-principles method to study near-field heat transfer mediated by Coulomb interaction,” *Phys. Rev. B* **104**, L121409 (2021).
- 250.** H. Zhou, G. Zhang, J.-S. Wang, Y.-W. Zhang, “Quantum mechanical exploration of anharmonic phonon transport across a weakly interacting interface,” submitting.
- 251.** Z.-Q. Zhang and J.-S. Wang, “Electroluminescence and thermal radiation from metallic carbon nanotubes with defects,” *Phys. Rev. B*, **104**, 085422 (2021).
- 252.** G. Liu, Z. Zhang, H. Wang, G. Li, J.-S. Wang, and Z. Gao, “Large contribution of quasi-acoustic shear phonon modes to thermal conductivity in novel monolayer Ga₂O₃,” *J. Appl. Phys.* **130**, 105106 (2021).