Chun-Wei Pao, Ph.D.

cwpao@gate.sinica.edu.tw https://www.linkedin.com/in/cwpao/
https://goo.gl/P2K8kV

Education

2004 – 2007 **Ph.D., Princeton University, USA** Department of Mechanical and Aerospace Engineering.
Thesis title: *Atomistic simulation of stress evolution during thin film growth.*

2002 – 2004 **M.A., Princeton University, USA** Department of Mechanical and Aerospace Engineering.

1999 – 2001 **M.S. National Taiwan University, Taiwan** in Institute of Applied Mechanics
Thesis title: *A study of classical and quantum Monte Carlo methods and their applications.*

1992 – 1996 **B.A. National Tsing Hua University, Taiwan** in Department of Power Mechanical Engineering

Research Experiences

2018 – · · · · **Research Fellow,** Research Center for Applied Sciences, Academia Sinica, Taiwan.

2020 – · · · · **Adjunct Professor,** Department of Photonics, National Yang Ming Chiao Tung University, Taiwan.

2018 – · · · · **Joint Professor,** Department of Matererials Science and Engineering, National Dong Hwa University, Taiwan.

2014 – 2018 **Associate Research Fellow,** Research Center for Applied Sciences, Academia Sinica, Taiwan.

2009 – 2014 **Assistant Research Fellow,** Research Center for Applied Sciences, Academia Sinica, Taiwan.

2007 – 2009 **Post-doctoral Research Associate,** Theoretical Division, Los Alamos National National Laboratory, USA.

2006 – 2006 **NECIS Summer Program Visiting Graduate Student,** Sandia National Laboratories, Albuquerque, USA.

1998 – 1999 **Research Assistant,** Magnet Group, Synchrotron Radiation Research Center, Taiwan.

Awards and Honors

2023 **Y.Z. Hsu Science Paper Award**

2022 **Investigator Award,** Academia Sinica.

2018 **IUPAC Distinguished Award for Novel Materials and their Synthesis**

2015 **Career Development Award,** Academia Sinica.

2014 **Youth Award**.

Young Theorist Award, National Center for Theoretical Sciences.

2013 **Project for Excellent Junior Research Investigators,** National Science Council of Taiwan.

Awards and Honors (continued)

2001 **Honorary membership of Phi Tau Phi Honor Society**, National Taiwan University.

Research Publications

Journal Articles

1. P.-Y. Yang, Y.-H. Chiang, C.-W. Pao, and C.-C. Chang, "Hybrid Machine Learning-Enabled Potential Energy Model for Atomistic Simulation of Lithium Intercalation into Graphite from Plating to Overlithiation", en, Journal of Chemical Theory and Computation.
2. Y.-H. Wang, C.-H. Yeh, I.-T. Hsieh, P.-Y. Yang, Y.-W. Hsiao, H.-T. Wu, C.-W. Pao, and C.-F. Shih, "Comparative Study of the Orientation and Order Effects on the Thermoelectric Performance of 2D and 3D Perovskites", en, Nanomaterials **14**, 446 (2024).
3. Y.-T. Chuang, T.-Y. Lin, G.-H. Tan, P.-E. Jan, H.-C. Lin, H.-M. Chen, K.-Y. Hsiao, B.-H. Chen, C.-H. Lu, C.-H. Lee, C.-W. Pao, S.-D. Yang, M.-Y. Lu, and H.-W. Lin, "Highly Efficient $MAPbI_3$ -Based Quantum Dots Exhibiting Unusual Nonblinking Single Photon Emission at Room Temperature", en, Small, 2308676 (2023).
4. B.-H. Lin, Y.-C. Chao, I.-T. Hsieh, C.-P. Chuu, C.-J. Lee, F.-H. Chu, L.-S. Lu, W.-T. Hsu, C.-W. Pao, C.-K. Shih, J.-J. Su, and W.-H. Chang, "Remarkably Deep Moiré Potential for Intralayer Excitons in MoSe2/MoS2 Twisted Heterobilayers", Nano Letters **23**, Publisher: American Chemical Society, 1306–1312 (2023).
5. R. Paste, C. Hanmandlu, P.-Y. Su, C.-H. Hou, H.-A. Chen, C.-W. Pao, J.-J. Shyue, K.-H. Chen, H.-L. Wu, H.-C. Lin, and C. W. Chu, "Intimate interaction of TFSI anions with MoO3x oxygen vacancies boost ionic conductivity of cathode-supported solid polymer electrolyte", Chemical Engineering Journal **452**, 139088 (2023).
6. S. A. Abbas, H.-A. Chen, A. Mohapatra, A. Singh, S. Li, C.-W. Pao, and C. W. Chu, "Sweetening Lithium Metal Interface by High Surface and Adhesive Energy Coating of Crystalline - d -Glucose Film to Inhibit Dendrite Growth", en, Small **18**, 2201349 (2022).
7. C. Hanmandlu, M. Sahoo, C.-C. Liu, H.-A. Chen, C.-W. Pao, Y.-C. Chang, C.-W. Chu, and C.-S. Lai, "Few-layer fluorine-functionalized graphene hole-selective contacts for efficient inverted perovskite solar cells", Chemical Engineering Journal **430**, 132831 (2022).
8. Q. F. He, J. G. Wang, H. A. Chen, Z. Y. Ding, Z. Q. Zhou, L. H. Xiong, J. H. Luan, J. M. Pelletier, J. C. Qiao, Q. Wang, L. L. Fan, Y. Ren, Q. S. Zeng, C. T. Liu, C. W. Pao, D. J. Srolovitz, and Y. Yang, "A highly distorted ultraelastic chemically complex Elinvar alloy", en, Nature **602**, 251–257 (2022).
9. P.-C. Hsu, Y.-C. Lin, W.-H. Wu, C.-W. Pao, and C.-H. Chen, "Atomistic Investigation of Solid Electrolyte Interphase: nanostructure, Chemical Composition and Mechanical Properties", en, Journal of The Electrochemical Society **169**, Publisher: IOP Publishing, 120520 (2022).
10. L.-Y. Su, H.-H. Huang, C.-E. Tsai, C.-H. Hou, J.-J. Shyue, C.-H. Lu, C.-W. Pao, M.-H. Yu, L. Wang, and C.-C. Chueh, "Improving Thermal and Photostability of Polymer Solar Cells by Robust Interface Engineering", en, Small **18**, 2107834 (2022).
11. F. Baskoro, H. Q. Wong, K. B. Labasan, C.-W. Cho, C.-W. Pao, P.-Y. Yang, C.-C. Chang, C.-I. Chen, C.-C. Chueh, W. Nie, H. Tsai, and H.-J. Yen, "An Efficient and Reversible Battery Anode Electrode Derived from a Lead-Based Metal–Organic Framework", en, Energy & Fuels **35**, 9669–9682 (2021).
12. C. H. Chen and **C. W. Pao**, "Phase-field study of dendritic morphology in lithium metal batteries", Journal of Power Sources **484**, Publisher: Elsevier B.V., 229203 (2021).

13. H.-a. Chen, P.-h. Tang, G.-j. Chen, C.-c. Chang, and C.-w. Pao, "Microstructure Maps of Complex Perovskite Materials from Extensive Monte Carlo Sampling Using Machine Learning Enabled Energy Model", 10.1021/acs.jpclett.1c00410 (2021).

14. Q. F. He, P. H. Tang, H. A. Chen, S. Lan, J. G. Wang, J. H. Luan, M. Du, Y. Liu, C. T. Liu, C. W. Pao, and Y. Yang, "Understanding chemical short-range ordering/demixing coupled with lattice distortion in solid solution high entropy alloys", Acta Materialia **216**, 117140 (2021).

15. S. Najman, H.-A. Chen, H.-Y. T. Chen, and C.-W. Pao, "Structural and Electronic Properties of Intertwined Defect in Ruddlesden–Popper 2D Perovskites Study Using Density Functional Theory Calculations", en, Multiscale Science and Engineering **3**, 205–215 (2021).

16. P.-Y. Yang and C.-W. Pao, "Molecular Simulations of the Microstructure Evolution of Solid Electrolyte Interphase during Cyclic Charging/Discharging", ACS Applied Materials & Interfaces, 10.1021/acsami.0c18783 (2021).

17. H.-A. Chen, P.-H. Lee, and C.-W. Pao, "Atomistic Structures and Energetics of Perovskite Nucleation Pathway During Sequential Deposition Process", Multiscale Science and Engineering **2**, Publisher: Springer Singapore, 227–234 (2020).

18. C. Hanmandlu, S. Swamy, A. Singh, Hsin-An Chen, C. C. Liu, C. S. Lai, A. Mohapatra, **C. W. Pao**, P. Chen, and C. W. Chu, "Suppression of surface defects to achieve hysteresis-free inverted perovskite solar cells: Via quantum dot passivation", Journal of Materials Chemistry A **8**, Publisher: Royal Society of Chemistry, 5263–5274 (2020).

19. N. Kaisar, A. Singh, P. Y. Yang, Y. T. Chen, S. Li, **C. W. Pao**, S. Jou, and C. W. Chu, "Long-lifespan lithium-metal batteries obtained using a perovskite intercalation layer to stabilize the lithium electrode", Journal of Materials Chemistry A **8**, Publisher: Royal Society of Chemistry, 9137–9145 (2020).

20. S. Najman, H.-A. Chen, H.-Y. Chen, and C.-W. Pao, "Surface structures and equilibrium shapes of layered 2D Ruddlesden-Popper perovskite crystals from density functional theory calculations", Materials Today Communications, 10.1016/j.mtcomm.2020.101745 (2020).

21. A. Singh, S. Najman, A. Mohapatra, Y. J. Lu, C. Hanmandlu, **C. W. Pao**, Y. F. Chen, C. S. Lai, and C. W. Chu, "Modulating Performance and Stability of Inorganic Lead-Free Perovskite Solar Cells via Lewis-Pair Mediation", ACS Applied Materials and Interfaces **12**, 32649–32657 (2020).

22. P. H. Tang, P. H. Chen, F. C. Li, C. H. Lu, C. I. Huang, and **C. W. Pao**, "Multiscale molecular simulations of the morphological evolution of small-molecule organic solar cells during the vacuum codeposition process", Physical Review Materials **4**, Publisher: American Physical Society, 1–12 (2020).

23. C. W. Tseng, D. C. Huang, H. L. Yang, H. C. Lin, F. C. Li, **C. W. Pao**, and Y. T. Tao, "Self-Assembly Behavior of Diacetylenic Acid Molecules upon Vapor Deposition: Odd–Even Effect on the Film Morphology", Chemistry - A European Journal **26**, 13948–13956 (2020).

24. H. A. Chen and **C. W. Pao**, "Fast and Accurate Artificial Neural Network Potential Model for MAPbI3 Perovskite Materials", ACS Omega **4**, 10950–10959 (2019).

25. K. C. Chen, L. M. Lee, H. A. Chen, H. Sun, C. L. Wu, H. A. Chen, K. B. Lin, Y. C. Tseng, C. C. Kaun, **C. W. Pao**, and S. Y. Lin, "Multi-layer elemental 2D materials: Antimonene, germanene and stanene grown directly on molybdenum disulfides", Semiconductor Science and Technology **34**, 10.1088/1361-6641/ab3c8a (2019).

26. Y.-T. Chen, S. Abbas, N. Kaisar, S. Wu, H.-A. Chen, K. Boopathi, M. Singh, J. Fang, C.-W. Pao, and C.-W. Chu, "Mitigating Metal Dendrite Formation in Lithium-Sulfur Batteries via Morphology-Tunable Graphene Oxide Interfaces", ACS Applied Materials and Interfaces **11**, 10.1021/acsami.8b18379 (2019).

27 N. Kaisar, S. A. Abbas, J. Ding, H. A. Chen, **C. W. Pao**, K. M. Boopathi, A. Mohapatra, Y. T. Chen, S. H. Wu, J. Fang, S. Jou, and C. W. Chu, "A lithium passivated MoO 3 nanobelt decorated polypropylene separator for fast-charging long-life Li-S batteries", Nanoscale **11**, 2892–2900 (2019).

28 Y.-X. Wang, H.-A. Chen, C.-W. Pao, and C.-C. Chang, "Artificial Neural Network Model for Atomistic Simulations of $${\rm {Sb/MoS}_{2}}$$ Sb / MoS 2 van der Waals Heterostructures", Multiscale Science and Engineering **1**, Publisher: Springer Singapore, 119–129 (2019).

29 H.-T. Wu, C.-W. Pao, Y.-C. Su, and C.-F. Shih, "Al-Doped ZnO/Silicon-rich Oxide Superlattices with High Room-Temperature Thermoelectric Figure of Merit", Materials Letters **245**, 10.1016/j.matlet.2019.02.063 (2019).

30 H.-T. Wu, Y.-C. Su, C.-W. Pao, and C.-F. Shih, "ZnO/Silicon-Rich Oxide Superlattices with High Thermoelectric Figure of Merit: A Comprehensive Study by Experiment and Molecular Dynamic Simulation", ACS Applied Materials and Interfaces **11**, 10.1021/acsami.8b20725 (2019).

31 H. A. Chen, H. Sun, C. R. Wu, Y. X. Wang, P. H. Lee, **C. W. Pao**, and S. Y. Lin, "Single-Crystal Antimonene Films Prepared by Molecular Beam Epitaxy: Selective Growth and Contact Resistance Reduction of the 2D Material Heterostructure", ACS Applied Materials and Interfaces **10**, 15058–15064 (2018).

32 C. L. Wu, H. T. Lin, H. A. Chen, S. Y. Lin, M. H. Shih, and **C. W. Pao**, "Defect formation and modulation during patterning supported graphene sheets using focused ion beams", Materials Today Communications **17**, Publisher: Elsevier, 60–68 (2018).

33 Y.-B. Lan, P.-H. Sher, C.-K. Lee, C.-W. Pao, C.-S. Tsao, Y.-C. Huang, P.-T. Huang, C.-I. Wu, and J.-K. Wang, "Revealing Ordered Polymer Packing during Freeze-Drying Fabrication of a Bulk Heterojunction Poly(3-hexylthiophene-2,5-diyl):[6,6]-Phenyl-C61-butyric Acid Methyl Ester Layer: In Situ Optical Spectroscopy, Molecular Dynamics Simulation, and X-ray Diffraction", The Journal of Physical Chemistry C **121**, Publisher: American Chemical Society, 14826–14834 (2017).

34 R. Valencia-Maturana and **C. W. Pao**, "Electronic and carrier transport properties of small molecule donors", Coupled Systems Mechanics **6**, 75–96 (2017).

35 C. L. Wu, F. C. Li, **C. W. Pao**, and D. J. Srolovitz, "Folding sheets with ion beams", Nano Letters **17**, Publisher: American Chemical Society, 249–254 (2017).

36 C. K. Lee and **C. W. Pao**, "Multiscale Molecular Simulation of Solution Processing of SMDPPEH: PCBM Small-Molecule Organic Solar Cells", ACS Applied Materials and Interfaces **8**, 20691–20700 (2016).

37 I. Amanatidis, J.-Y. Kao, L.-Y. Du, C.-W. Pao, and Y.-C. Chen, "Thermoelectric Efficiency of Single-Molecule Junctions: Phase Diagram Constructed from First-Principles Calculations", Journal of Physical Chemistry C **119**, 28728–28736 (2015).

38 C.-K. Lee, C.-W. Pao, and B. Smit, "PSII-LHCII supercomplex organizations in photosynthetic membrane by coarse-grained simulation", Journal of Physical Chemistry B **119**, 3999–4008 (2015).

39 M.-Y. Lin, C.-H. Wang, C.-W. Pao, and S.-Y. Lin, "Transferring-free and large-area graphitic carbon film growth by using molecular beam epitaxy at low growth temperature", Journal of Crystal Growth, 10.1016/j.jcrysgro.2015.02.039 (2015).

40 C.-W. W. Chen, Z.-Y. Y. Huang, Y.-M. M. Lin, W.-C. C. Huang, Y.-H. H. Chen, J. Strzalka, A. Y. Chang, R. D. Schaller, C.-K. K. Lee, C.-W. W. Pao, and H.-W. W. Lin, "Morphology, molecular stacking, dynamics and device performance correlations of vacuum-deposited small-molecule organic solar cells.", Physical chemistry chemical physics : {PCCP} **16**, 8852–8864 (2014).

41 C. K. Lee and **C. W. Pao**, "Nanomorphology evolution of p3ht/pcbm blends during solution-processing from coarse-grained molecular simulations", Journal of Physical Chemistry C **118**, ISBN: 1932-7447, 11224–11233 (2014).

42 C. K. Lee, O. Wodo, B. Ganapathysubramanian, and **C. W. Pao**, "Electrode materials, thermal annealing sequences, and lateral/vertical phase separation of polymer solar cells from multiscale molecular simulations", ACS Applied Materials and Interfaces **6**, 20612–20624 (2014).

43 T.-H. Liu, Y.-C. Chen, C.-W. Pao, and C.-C. Chang, "Anisotropic thermal conductivity of {MoS2} nanoribbons: Chirality and edge effects", Applied Physics Letters **104**, Publisher: {AIP} Publishing, 10.1063/1.4878395 (2014).

44 T. H. Liu, S. C. Lee, C. W. Pao, and C. C. Chang, "Anomalous thermal transport along the grain boundaries of bicrystalline graphene nanoribbons from atomistic simulations", Carbon **73**, 432 (2014).

45 T.-H. Liu, C.-W. Pao, and C.-C. Chang, "Mechanical mutability of polycrystalline graphene from atomistic simulations", Computational Materials Science **91**, 10.1016/j.commatsci.2014.04.031 (2014).

46 C.-K. Lee, C.-W. Pao, and C.-W. Chen, "Correlation of nanoscale organizations of polymer and nanocrystals in polymer/inorganic nanocrystal bulk heterojunction hybrid solar cells: insights from multiscale molecular simulations", Energy Environ. Sci. **6**, 307–315 (2013).

47 W.-H. Lin, K.-W. Wang, Y.-A. Liao, C.-W. Pao, and S.-Y. Lin, "The formation mechanisms and optical characteristics of GaSb quantum rings", Journal of Applied Physics **114**, 10.1063/1.4817419 (2013).

48 T.-H. Liu, C.-W. Pao, and C.-C. Chang, "Thermal response of grain boundaries in graphene sheets under shear strain from atomistic simulations", Computational Materials Science **70**, 10.1016/j.commatsci.2012.12.037 (2013).

49 T.-H. Liu, C.-W. Pao, and C.-C. Chang, "An analytical model for calculating thermal properties of two-dimensional nanomaterials", Applied Physics Letters **103**, 10.1063/1.4826693 (2013).

50 D. Patra, T.-Y. Huang, C.-C. Chiang, R. O. V. Maturana, C.-W. Pao, K.-C. Ho, K.-H. Wei, and C.-W. Chu, "2-Alkyl-5-thienyl-Substituted Benzo[1,2- *b* :4,5- *b*]dithiophene-Based Donor Molecules for Solution-Processed Organic Solar Cells", ACS Applied Materials & Interfaces **5**, 9494–9500 (2013).

51 B. Song, J. Jansen, F. D. Tichelaar, H. W. Zandbergen, G. Gajewski, C. W. Pao, and D. J. Srolovitz, "In-situ transmission electron microscopy and first-principles study of Au (100) surface dislocation dynamics", Surface Science **608**, 154 (2013).

52 C.-K. Lee and C.-W. Pao, "Solubility of [6,6]-phenyl-C <inf>61</inf>-butyric acid methyl ester and optimal blending ratio of bulk heterojunction polymer solar cells", Journal of Physical Chemistry C **116**, 10.1021/jp3028947 (2012).

53 W.-J. Lee, C.-W. Pao, and J.-G. Chang, "Helical multi-shell structures in gold nanobridge and suspending nanowire", Journal of Nanoparticle Research **14**, 10.1007/s11051-012-1058-3 (2012).

54 W.-J. Lee, C.-W. Pao, Y.-T. Wang, W.-S. Su, and J.-G. Chang, "Diffusion of the vacancy defect leading to the formation of multi-shell structures in the nanowire and nanobridge", Journal of Applied Physics **112**, 10.1063/1.4766406 (2012).

55 C.-C. Lin, P.-H. Ho, C.-L. Huang, C.-H. Du, C.-C. Yu, H.-L. Chen, Y.-C. Yeh, S.-S. Li, C.-K. Lee, C.-W. Pao, C.-P. Chang, M.-W. Chu, and C.-W. Chen, "Dependence of nanocrystal dimensionality on the polymer nanomorphology, anisotropic optical absorption, and carrier transport in P3HT:TiO<inf>2</inf> bulk heterojunctions", Journal of Physical Chemistry C **116**, 10.1021/jp306921e (2012).

56 M.-Y. Lin, W.-C. Guo, M.-H. Wu, P.-Y. Wang, T.-H. Liu, C.-W. Pao, C.-C. Chang, S.-C. Lee, and S.-Y. Lin, "Low-temperature grown graphene films by using molecular beam epitaxy", Applied Physics Letters **101**, 10.1063/1.4768948 (2012).

57 T.-H. Liu, C.-W. Pao, and C.-C. Chang, "Effects of dislocation densities and distributions on graphene grain boundary failure strengths from atomistic simulations", Carbon (2012).

58 C.-W. Pao, T.-H. Liu, C.-C. Chang, and D. J. Srolovitz, "Graphene defect polarity dynamics", Carbon (2012).

59 G. Gajewski and C.-W. Pao, "Ab Initio Calculations of the Reaction Pathways for Methane Decomposition Over the Cu (111) Surface", Journal of Chemical Physics **135**, 064707 (2011).

60 C.-K. Lee, C.-W. Pao, and C.-W. Chu, "Multiscale molecular simulations of the nanoscale morphologies of P3HT:PCBM blends for bulk heterojunction organic photovoltaic cells", Energy & Environmental Science **4**, 4124 (2011).

61 C.-W. Pao, S. Foiles, E. Webb, D. Srolovitz, and J. Floro, "Atomistic simulations of stress and microstructure evolution during polycrystalline Ni film growth", Physical Review B **79**, 1–9 (2009).

62 C.-W. Pao and D. J. Srolovitz, "Compressive film stress in a thin, tensile heteroepitaxial film", Applied Physics Letters **93**, 011903 (2008).

63 C.-W. Pao, S. Foiles, E. Webb, D. Srolovitz, and J. Floro, "Thin Film Compressive Stresses due to Adatom Insertion into Grain Boundaries", Physical Review Letters **99**, 1–4 (2007).

64 C.-W. Pao, D. Srolovitz, and H. Zandbergen, "Thermodynamic and kinetic properties of surface dislocations on Au(001) from atomistic simulations", Physical Review B **75**, 1–11 (2007).

65 H. Zandbergen, C.-W. Pao, and D. Srolovitz, "Dislocation Injection, Reconstruction, and Atomic Transport on {001} Au Terraces", Physical Review Letters **98**, 1–4 (2007).

66 C.-W. Pao and D. Srolovitz, "Stress and Morphology Evolution during Island Growth", Physical Review Letters **96**, 1–4 (2006).

67 C.-W. Pao, D. Srolovitz, and C. Thompson, "Effects of surface defects on surface stress of Cu(001) and Cu(111)", Physical Review B **74**, 1–8 (2006).

68 C.-W. Pao and D. J. Srolovitz, "Atomistic simulation of stress evolution during island growth", Journal of the Mechanics and Physics of Solids **54**, 2527–2543 (2006).