Maria Chan

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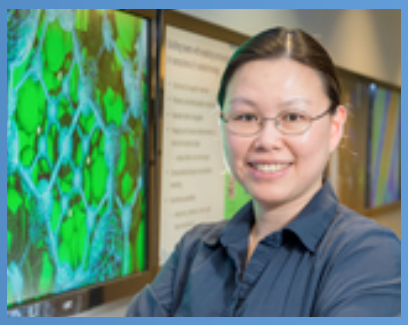

Education

Ph. D. Physics, Massachusetts Institute of Technology
B. S. Physics & Applied Mathematics, University of California, Los Angeles

Research Interests

Development of efficient atomistic and first principles computation methodologies, and application of such to renewable energy materials and nanoscale phenomena. Research topics include first principles and atomistic modeling of nanomaterials and renewable energy materials, e.g. photovoltaics, energy storage, photo- and electro-catalysts, thermal transport, and thermoelectrics. Also involved in methodology and software development for integrating atomistic modeling and experimental measurements.

Professional Experience

Argonne National Laboratory - Center for Nanoscale Materials ***2012-present***
Assistant Scientist

- Center for Nanoscale Materials: structural and electronic properties of semiconductor nanoparticles, transition-metal dichalcogenides for catalysis, hybrid perovskite photovoltaics, force field development, connecting modeling to synchrotron characterization and microscopy techniques using machine learning
- Center for Electrochemical Energy Science: high capacity lithium-ion, lithium-oxygen, and hybrid lithium-ion/lithium-oxygen battery materials, solid-electrolyte interphase, surface and interfacial interactions
- Midwest Integrated Center for Computational Materials: validation of computational software for materials modeling
- DOE SunShot: grain boundaries in CdTe photovoltaics
- Industrial sponsors: electronic and lattice thermal transport modeling

Argonne National Laboratory - Center for Nanoscale Materials & Center for Electrical Energy Storage ***2010-2012***
Postdoctoral Associate

- Si as anodes for Li-ion batteries: developed algorithm to simulate lithiation and delithiation of crystalline silicon; investigated effects of surface orientation, dopants, and surface chemistry on thermodynamics and kinetics of Li-Si reaction. Investigated effects of micro- and nano-structuring on lithiation reaction.
- Transition metal oxide electrocatalysts for Li-air batteries: investigated Fe and Mn oxides capable of incorporating Li-oxides in their structure; investigated oxygen reduction and evolution reaction in these transition metal oxides in Li/oxygen battery environment.

Massachusetts Institute of Technology - Materials Science & Engineering ***2009-2010***
Postdoctoral Associate

- High-throughput search for novel materials for solar energy conversion: defect studies, band edge level predictions in aqueous environment, effects of interfacial phase stability/electronic structures and defects on photovoltaic performance.
- Correlation effects in transition metal oxides and halides: evaluated DFT+U and hybrid functionals for the accurate computation of formation and redox energies.

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Publications

Method development

1. B. Narayanan, A. Kinaci, M. J. Davis, S. K. Gray, M. K. Y. Chan, and S. K. R. S. Sankaranarayanan, "Describing the diverse geometries of gold from nanoclusters to bulk – a first principles based hybrid bond order potential," Journal of Physical Chemistry C, accepted (2016).
2. F. G. Sen, A. Kinaci, B. Narayanan, M. J. Davis, S. Gray, S. Sankaranarayanan, and M. Chan, "Towards accurate prediction of catalytic activity in IrO_2 nanoclusters via first principles-based variable charge force field," Journal of Materials Chemistry A **3**, 18970 (2015). DOI:10.1039/C5TA04678E. Featured on PhysOrg, May 2016.
3. Z. Zeng, M. K. Y. Chan, and J. P. Greeley, "Towards first-principles based prediction of highly accurate electrochemical Pourbiax diagrams," Journal of Physical Chemistry C **119**, 18177 (2015). DOI:10.1021/acs.jpcc.5b03169.
4. A. Knoll, M. K. Y. Chan, K. C. Lau, B. Liu, J. P. Greeley, L. Curtiss, M. Hereld, M. E. Papka, "Uncertainty Classification and Visualization of Molecular Surfaces," International Journal for Uncertainty Quantification **3**, 157 (2013). DOI: 10.1615/Int.J.UncertaintyQuantification.2012003950.
5. Y. B. Wu, M. K. Y. Chan, and G. Ceder, "Prediction of semiconductor band edge positions in aqueous environments from first principles," Physical Review B **83**, 235301 (2011).
6. M. K. Y. Chan and G. Ceder, "Efficient band gap prediction in solids," Physical Review Letters **105**, 196403 (2010). DOI: 10.1103/PhysRevLett.105.196403. Editors' suggestion. Featured on PhysOrg, November 2010.
7. V. L. Chevrier, S. P. Ong, R. Armiento, M. K. Y. Chan, and G. Ceder, "Hybrid density functional calculations of redox potentials and formation energies of transition metal compounds," Physical Review B **82**, 075122 (2010). DOI: 10.1103/PhysRevB.82.075122.

Electrochemistry, Energy Storage, and Electrocatalysis

1. H. Yildirim,* A. Kinaci,* M. K. Y. Chan, and J. P. Greeley, "First Principles Analysis of Defect Thermodynamics and Ion Transport in Inorganic SEI Compounds," ACS Applied Materials and Interfaces **7**, 18985 (2015). DOI:10.1021/acsami.5b02904. *Co-first-authors
2. M. R. Gao, M. K. Y. Chan, Y. Sun, "Edge-oriented molybdenum disulfide with expanded interlayers for electrochemical hydrogen production," Nature Communications **6**, 7493 (2015). DOI:10.1038/ncomms8493.
3. Z. Yang, L. Trahey, Y. Ren, M. K. Y. Chan,[#] C. Lin, J. Okasinski, and M. M. Thackeray, "In-Situ High-Energy Synchrotron X-ray Diffraction Studies and First Principles Modeling of α-MnO_2 Electrodes in Li-O_2 and Li-ion Coin Cells," Journal of Materials Chemistry A **3**, 7389 (2015). DOI:10.1039/C4TA06633B. #Corresponding author.
4. H. Yildirim, A. Kinaci, Z.-J. Zhao, M. K. Y. Chan, J. P. Greeley, "First-Principles Analysis of Defect-Mediated Li Adsorption on Graphene," ACS Applied Materials and Interfaces **6**, 21141 (2014). DOI:10.1021/am506008w.
5. B. Liu, M. Zhou, M. K. Y. Chan, and J. P. Greeley, "Understanding Glycerol Decomposition on Bimetallic PtMo Catalysts from First-principles Methods," ACS Catalysis **5**, 4942 (2015). DOI:10.1021/acscatal.5b01127.
6. L. Jaber-Ansari, K. Puntambekar, H. Tavassol, H. Yildirim, A. Kinaci, R. Kumar, S. Saldana, A. Gewirth, J. P. Greeley, M. K. Y. Chan, M. Hersam, "Defect Evolution in Graphene upon Electrochemical Lithiation," ACS Applied Materials and Interfaces **6**, 17626 (2014). DOI:10.1021/am503715g.
7. S. Kirklin, M. K. Y. Chan, L. Trahey, M. M. Thackeray, and C. Wolverton, "High-throughput screening of high-capacity electrodes for hybrid Li-ion/Li-O_2 cells," Physical Chemistry Chemical Physics **16**, 22073 (2014). DOI:10.1039/C4CP03597F.
8. K. C. Lau, L. A. Curtiss, M. K. Y. Chan, J. P. Greeley, "Atomistic and First Principles Computational Studies of Li-O_2 Batteries", in *Lithium air batteries*, Edited by P. Bruce, A. Luntz

and N. Imanishi, Springer 2014. http://www.springer.com/us/book/9781489980618.
9. M. M. Thackeray, M. K. Y. Chan, L. Trahey, S. Kirklin, and C. Wolverton, "Vision for Designing High-Energy, Hybrid Li Ion/Li-O_2 Cells," Journal of Physical Chemistry Letters **4**, 3607 (2013). DOI:10.1021/jz4018464.
10. H. Tavassol, M. K. Y. Chan, M. G. Catarello, J. P. Greeley, D. G. Cahill, and A. A. Gewirth, "Surface Coverage and SEI Induced Electrochemical Surface Stress Changes during Li Deposition in a Model System for Li-Ion Battery Anodes," Journal of the Electrochemical Society **160**, A888 (2013). DOI: 10.1149/2.068306jes.
11. L. Trahey, N. Karan, M. K. Y. Chan, J. Lu, Y. Ren, J. P. Greeley, M. Balasubramanian, A. K. Burrell, and M. M. Thackeray, "Synthesis, Characterization and Structural Modeling of High Capacity, Dual-Functioning MnO_2 Electrode/Electrocatalysts for Li-O_2 Batteries," Advanced Energy Materials **3**, 75 (2013). DOI:10.1002/aenm.201200037.
12. M. K. Y. Chan, C. Wolverton, and J. P. Greeley, "First Principles Simulations of the Electrochemical Lithiation and Delithiation of Faceted Crystalline Silicon," Journal of the American Chemical Society **134**, 14362 (2012). DOI:10.1021/ja301766z.
13. R. Subbaraman, D. Tripkovic, K. C. Chang, D. Strmcnik, A. P. Paulikas, P. Hirunsit, M. K. Y. Chan, J. P. Greeley, V. Stamenkovic, and N. M. Markovic, "Activity trends for the hydrogen and oxygen production on Pt(111) modified by Ni, Co, Fe and Mn (hydroxy)oxide clusters in alkaline environments," Nature Materials **11**, 550 (2012). DOI:10.1038/nmat3313.
14. T. Fister, M. Schmidt, C. S. Johnson, M. Slater, E. Shirley, M. K. Y. Chan and P. Fenter, "Electronic structures of lithium battery interphase compounds: comparison between inelastic x-ray scattering measurements and theory," Journal of Chemical Physics **135**, 224513 (2011). DOI:10.1063/1.3664620.
15. M. K. Y. Chan, B. Long, A. Gewirth and J. P. Greeley, "The first-cycle electrochemical lithiation of crystalline Ge – dopant and orientation dependence, and comparison with Si," Journal of Physical Chemistry Letters **2**, 3092 (2011). DOI:10.1021/jz201432d.
16. T. T. Truong, Y. Qin, Y. Ren, Z. Chen, M. K. Y. Chan, J. P. Greeley, K. Amine and Y. Sun, "Single-crystal silicon membranes with high lithium conductivity and application in lithium-air batteries," Advanced Materials **23**, 4947 (2011). DOI: 10.1002/adma.201102449.
17. M. K. Y. Chan, E. L. Shirley, N. K. Karan, M. Balasubramanian, J. P. Greeley, and T. Fister "Structure of lithium peroxide," Journal of Physical Chemistry Letters **2**, 2483, (2011). DOI: 10.1021/jz201072b.
18. B. Long, M. K. Y. Chan, J. P. Greeley and A. Gewirth, "Dopant Modulated Li Insertion in Si for Battery Anodes," Journal of Physical Chemistry C **115**, 18916 (2011). DOI: 10.1021/jp2060602.

Photovoltaics

1. C. Sun*, T. Paulauskas*, F. G. Sen*, G. Lian, J. Wang, C. Buurma, M. K. Y. Chan, R. F. Klie, and M. J. Kim, "Atomic and electronic structure of Lomer dislocations at CdTe bicrystal interface," Scientific Reports, accepted (2016). *Equal contributions.
2. A. Y. Chang, Y.-J. Cho, K.-C. Chen, C.-W. Chen, A. Kinaci, M. K. Y. Chan, H.-W. Lin, R. D. Schaller, "Evidence of Slow Organic-to-Inorganic Sub-Lattice Thermalization in Methylammonium Lead Halide Perovskites," Advanced Energy Materials, accepted (2016).
3. T. Paulauskas, C. Buurma, B. Stafford, C. Sun, M. K. Y. Chan, Sivananthan Sivalinghama, M. J. Kim and R. F. Klie, "Atomic Scale Study of Lomer-Cottrell and Hirth Lock Dislocations in CdTe," Microscopy and Microanalysis **21**, 2087 (2015). DOI: 10.1017/S1431927615011216.
4. T. Paulauskas, C. Buurma, C. Sun, M. K. Y. Chan, M. J. Kim, F. G. Sen, R. F. Klie, "A Fundamental Study of the Effects of Grain Boundaries on Performance of Poly-Crystalline Thin Film CdTe Solar Cells," Proceedings of the 42nd IEEE Photovoltaic Specialists Conference (PVSC), (2015). DOI: 10.1109/PVSC.2015.7355937.
5. C. Buurma, F. G. Sen, T. Paulauskas, C. Sun, M. J. Kim, S. Sivananthan, R. F. Klie, M. K. Y. Chan, "Creation and Analysis of Atomic Structures for CdTe Bi-crystal Interfaces by the Grain

Boundary Genie," Proceedings of the 42nd IEEE Photovoltaic Specialists Conference (PVSC), (2015). DOI: 10.1109/PVSC.2015.7355936.
6. F. G. Sen, C. Buurma, T. Paulauskas, C. Sun, M. J. Kim, S. Sivananthan, R. F. Klie, M. K. Y. Chan, "Atomistic simulations of grain boundaries in CdTe," Proceedings of the 42nd IEEE Photovoltaic Specialists Conference (PVSC), (2015). DOI:10.1109/PVSC.2015.7355935
7. K. Pelzer, M. K. Y. Chan, S. Gray, S. Darling, "Polaron Structure and Transport in Fullerene Materials: Insights from First-Principles Calculations," Journal of Physical Chemistry C **118**, 21785 (2014). DOI:10.1021/jp504923x.
8. T. Paulauskas, C. Buurma, E. Colegrove, B. Stafford, Z. Guo, M. K. Y. Chan, C. Sun, M. Kim, S. Sivananthan and R. Klie, "Atomic-scale study of polar Lomer-Cottrell and Hirth lock dislocation cores in CdTe," Acta Crystallographica Section A **70**, 524 (2014). DOI:10.1107/S2053273314019639.
9. T. Paulauskas, C. Buurma, E. Colegrove, Z. Guo, S. Sivananthan, M. K. Y. Chan, R. F. Klie, "Atomic-resolution characterization of the effects of $CdCl_2$ treatment of poly-crystalline CdTe thin films," Applied Physics Letters **105**, 071910 (2014). DOI:10.1063/1.4893727.
10. P. Lazic, R. Armiento, W. F. Herbert, R. Chakraborty, R. Sun, M. K. Y. Chan, K. Hartman, T. Buonassisi, B. Yildiz, K. J. Van Vliet, and G Ceder, "Low Intensity Conduction States in FeS_2: Implications for Absorption, Open-Circuit Voltage and Surface Recombination," Journal of Physics: Condensed Matter **25**, 465801 (2013). DOI:10.1088/0953-8984/25/46/465801.
11. R. S. Sun, M. K. Y. Chan, S. Y. Kang, and G. Ceder, "Intrinsic stoichiometry and oxygen-induced p-type conductivity of pyrite FeS_2," Physical Review B **84**, 035212 (2011). DOI: 10.1103/PhysRevB.84.035212.
12. R. S. Sun, M. K. Y. Chan, and G. Ceder, "First-principles electronic structure and relative stability of pyrite and marcasite: Implications for photovoltaic performance," Physical Review B **83**, 235311 (2011). DOI: 10.1103/PhysRevB.83.235311.

Nanoparticles

1. Y. A. Wu, L. Li, Z. Li, A. Kinaci, M. K. Y. Chan, Y. Sun, J. R. Guest, I. McNulty, T. Rajh, Y. Liu, "Visualizing Redox Dynamics of a Single Ag/AgCl Heterogeneous Nanocatalyst at Atomic Resolution," ACS Nano 10, 3738 (2016). DOI:10.1021/acsnano.6b00355.
2. C. E. Rowland, W. Liu, D. C. Hannah, M. K. Y. Chan, D. V. Talapin, R. D. Schaller, "Thermal Stability of Colloidal InP Nanocrystals: Small Inorganic Ligands Boost High-Temperature Photoluminescence," ACS nano **8**, 977 (2013). DOI:10.1021/nn405811p.
3. D. C. Hannah, J. Yang, P. Podsiadlo, M. K. Y. Chan, D. Gosztola, V. Prakapenka, G. Schatz, U. Kortshagen, R. Schaller, "On the Origin of Photoluminescence in Silicon Nanocrystals: Pressure-Dependent Structural and Optical Studies," Nanoletters **12**, 4200 (2012). DOI:10.1021/nl301787g.

Thermal transport

1. Kinaci, M. Kado, D. Rosenmann, C. Ling, G. Zhu, D. Banerjee, M. K. Y. Chan, "Electronic Transport in VO_2 – Experimentally-Calibrated Boltzmann Transport Modeling," Applied Physics Letters **107**, 262108 (2015). DOI:10.1063/1.4938555.
2. M. K. Y. Chan, J. Reed, D. Donadio, T. Mueller, Y. S. Meng, G. Galli, and G. Ceder, "Cluster expansion and optimization of thermal conductivity in SiGe nanowires," Physical Review B **81**, 174303 (2010). Editors' suggestion. DOI: 10.1103/PhysRevB.81.174303.