Dr Maria K Y Chan
Center for Nanoscale Materials
Argonne National Laboratory
9700 S. Cass Ave, Argonne IL 60439, USA
Office: (630) 252-4811 Cell: (617) 407-0842 E-mail: mchan@anl.gov
Website: http://www.anl.gov/cnm/person/maria-k-y-chan

Education

Massachusetts Institute of Technology, Cambridge MA, USA
PhD in Physics | Thesis: "Atomistic and *Ab Initio* Prediction and Optimization of Thermoelectric and Photovoltaic Properties" | Advisor: Professor Gerbrand Ceder
University of California, Los Angeles, Los Angeles CA, USA
BSc in Physics and Applied Mathematics

Expertise

Computational prediction of materials properties, using first principles, atomistic, and data mining methods, particularly in applications towards materials relevant to energy technologies. Building effective physical models for computationally-efficient predictions and optimization.

Appointments

- University of Chicago, Computation Institute, Fellow, 2014-present
- Argonne National Laboratory, Center for Nanoscale Materials, Assistant Scientist, 2012-present
- Argonne National Laboratory, Center for Nanoscale Materials and Center for Electrical Energy Storage (DOE Energy Frontier Research Center), Postdoctoral Associate, 2010-2012
- Massachusetts Institute of Technology, Department of Materials Science and Engineering, Postdoctoral Associate, 2009-2010

Funding

- Center for Nanoscale Materials, DOE Office of Science
- Center for Electrochemical Energy Science (CEES) EFRC, DOE Office of Science
- Midwest Integrated Center for Computational Materials, DOE Office of Science
- SunShot BRIDGE, DOE Office of Energy Efficiency and Renewable Energy
- Strategic Partnership Project with Toyota Research Institute of North America
- Argonne Laboratory Directed Research & Development grants

Selected Publications

(Full list at http://scholar.google.com/citations?hl=en&user=ZXmeZrwAAAAJ)

- 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.
- F. G. Sen, 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.
- 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.
- 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.
- 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.
- 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.

- 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.
- 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.
- 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.
- 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.
- 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.
- 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.
- 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).
- 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.
- 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).

Selected Invited Talks

- "Non-equilibrium configurational sampling and predictive modeling of renewable energy materials," Physics Department, Hong Kong University of Science and Technology, Hong Kong, December 2015.
- "Hybrid Li-Ion/Li-Oxygen Battery Materials" Electrochemical Society Fall Meeting, Phoenix AZ, October 2015.
- "Hybrid Li-Ion/Li-Oxygen Battery Materials – a First Principles Perspective," Materials Science and Engineering, University of California, Santa Barbara CA, September 2015.
- "Non/Near-Equilibrium configurational sampling," Telluride Workshop on Computational Materials Chemistry, Telluride CO, June 2015.
- "Density functional theory modeling of twin boundaries in CdTe as informed by STEM observations," Microscopy and Microanalysis, Hartford CT, August 2014.
- "First principles atomistic modeling of surface and interfacial effects in lithium ion battery materials," American Chemical Society Spring Meeting, New Orleans LA, April 2013.

Synergistic Activities

- Organizer of the "Materials for Energy Storage" focus session at the American Physical Society March 2014 meeting, and the "In Silico Materials Chemistry" symposium at the Materials Research Society 2016 Fall Meeting.
- Organizer of the "Solar Energy Capture and Conversion at the Nanoscale" and "Experimental and Computational Challenges of *in situ* Multimodal Imaging of Energy Materials" workshops at the APS/CNM/EMC Users Meetings at Argonne National Lab.
- Participant in Expanding Your Horizons Chicago, Science Careers in Search of Women, and other outreach events aimed at increasing the participation of minorities and women in STEM fields, ongoing.