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Research Summary:

Current research focuses on the computational prediction of materials properties, using first principles, atomistic, and data mining methods, particularly in applications towards materials relevant to energy technologies, such as photovoltaics, energy storage, and thermoelectrics. Examples include development of methods for high-throughput screening of photovoltaic and photocatalytic materials, prediction of thermal conductivity in nanostructured thermoelectric materials, and modeling of high-capacity electrode materials for lithium ion and lithium air batteries. Currently funded as a PI in the [Center for Electrical Energy Storage](#), a DOE EFRC, and a [DOE Sunshot](#) project on grain boundaries in CdTe.

Selected Publications: ([Google scholar](#))

M. K. Y. Chan, C. Wolverton, and J. Greeley, "First Principles Simulations of the Electrochemical Lithiation and Delithiation of Faceted Crystalline Silicon," *Journal of the American Chemical Society*, **134**, 14362 (2012).

M. K. Y. Chan, B. Long, A. Gewirth and J. 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).

Yabi 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).

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).

M. K. Y. Chan and G. Ceder, "Efficient band gap prediction in solids," *Physical Review Letters*, **105**, 196403 (2010). Editors' suggestion.

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.