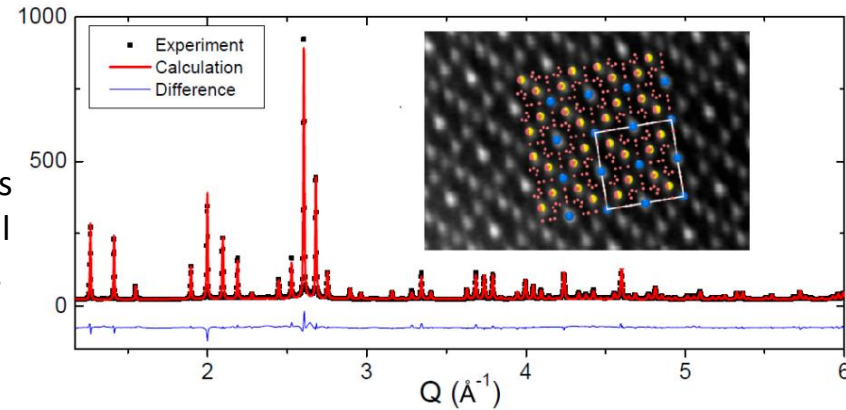


Adaptive Genetic Algorithm and Motif Search for Material Discovery and Material Informatics

Scientific achievements and impacts:

Solving crystal structure of complex intermetallic compounds

- ϵ -AlSm has a unit cell ~ 140 atoms and with disordered anti-sites defects. Results reveal a topological connection between crystal and undercooled liquids and amorphous systems. [Z. Ye, F Zhang, Y. Sun, M. C. Nguyen, S. H. Zhou, L. Zhou, F. Meng, R. T. Ott, E. Park, M. F. Besser, M. J. Kramer, Z. J. Ding, M. I. Mendeleev, C. Z. Wang, R. E. Napolitano and K. M. Ho, *Phys. Rev. Mater.* accepted]



Advanced structure space sampling method: Application to battery cathode materials

- Motif search and adaptive genetic algorithm methods enable great expansion of existing structural databases. As a demonstration, we constructed a more comprehensive structure database for LiFePO_4 with an 8-fold increase in low-energy structures. [X. B. Lv, X. Zhao, S. Wu, P. Wu, Y. Wang, M. C. Nguyen, Y. Shi, Z. Lin, C. Z. Wang and K. M. Ho, *J. Mater. Chem. A* **5**, 14611 (2017)]

Solving structural puzzle of permanent magnet materials

- Complex structures of the $\text{Zr}_2\text{Co}_{11}$ polymorphs (up to 150 atoms/cell) are resolved using the adaptive genetic algorithm, allowing us to elucidate the physical origin of high coercivity in this rare-earth-free permanent magnetic system. [X. Zhao, M. C. Nguyen, W. Zhang, C. Z. Wang, M. J. Kramer, D. J. Sellmyer, X. Li, F. Zhang, L. Ke, V. P. Antropov, and K. M. Ho, *Phys. Rev. Lett.* **112**, 045502 (2014)]

Photovoltaic and thermoelectric materials

- Solving the crystal structures of Cu_2X compounds ($\text{X} = \text{Te}, \text{Se}$ and S) provides useful insights into the Cu_2Te /semiconductor interfaces in thin-film solar cells and offers new opportunities for improving the thermoelectric properties of Cu_2Se . [M. C. Nguyen, J.-H. Choi, X. Zhao, C. Z. Wang, Z. Zhang and K. M. Ho, *Phys. Rev. Lett.* **111**, 165502 (2013)]

Future Directions: Material Informatics

