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Accelerating the exploration of Li/Na-ion battery materials via enlarged crystal structure databases

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Material informatics is a new initiative which has attracted a lot of attention in recent scientific research. The basic strategy is to construct comprehensive data sets and use machine learning to solve a wide variety of problems in material design and discovery. In pursuit of this goal, a key element is the quality and completeness of the databases used. Recent advance in the development of crystal structure prediction algorithms has made it a complementary and more efficient approach to explore the structure/phase space in materials using computers. In this talk, we discuss the importance of the structural motifs and motif-networks in crystal structure predictions. Correspondingly, powerful methods are developed to improve the sampling of the low-energy structure landscape. Applications to the Li/Na-ion battery cathode materials, in particular A_nFeSiO_4 (n=1 and 2; A=Li and Na) and $LiFePO_4$, will be presented.

References

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Biography

Kai-Ming Ho has completed his PhD from University of California, Berkeley. He is currently a Distinguished Professor in Liberal Arts and Sciences at Iowa State University and a Fellow of American Physical Society.

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