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第14回/1　情報統合型研究交流会

Machine Learning for Materials Discovery: Virtual screening and Bayesian optimization

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2016

4/20 15:00 – 15:45

東京大学柏キャンパス
総合研究棟6階大会議室

The scientific process of discovering new knowledge is often characterized as search from a space of candidates, and machine learning can accelerate the search by properly modelling the data and suggesting which candidates to apply experiments on. In many cases, experiments can be substituted by first principles calculation. I review two basic machine learning techniques called virtual screening and Bayesian optimization for fast discovery. The power of this approach is exemplified by two of our recent studies. One is discovery of compounds of low lattice thermal conductivity from the materials project database. The other is fast determination of atomic structure of a crystalline interface.

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