Machine Learning Ab Initio Calculations for Materials Science

Shyue Ping Ong[1], Chi Chen[1], Xiangguo Li[1], Zhi Deng[1], Yunxing Zuo[1]

[1] University of California, San Diego, 9500 Gilman Dr. Mail Code #0448, La Jolla, CA 92093-0448

As unprecedented amounts of materials data generated from high-throughput ab initio calculations, machine learning techniques has the potential to greatly accelerate materials discovery and design. In this talk, I will present our latest efforts at developing high-accurate surrogate models for energies, forces and materials properties by machine learning "large" ab initio data. I will discuss various representations for crystals – from undirected graphs to local atomic density functions – and demonstrate how models built on these representations – from simple linear models to state-of-the-art graph networks – can achieve near-DFT accuracy in energy, force and property predictions. [1–5] Finally, I outline how such models may be used in accessing compositional, time and length scales far beyond that accessible by *ab initio* calculations today, enabling the search for novel materials in vast compositional spaces and the study of microstructure of materials.

References

[1] C. Chen, Z. Deng, R. Tran, H. Tang, I.-H. Chu, and S. P. Ong, Phys. Rev. Mater. **1**, 043603 (2017).
[2] X.-G. Li, C. Hu, C. Chen, Z. Deng, J. Luo, and S. P. Ong, Phys. Rev. B **98**, 094104 (2018).
[3] W. Ye, C. Chen, Z. Wang, I.-H. Chu, and S. P. Ong, Nat. Commun. **9**, 3800 (2018).
[4] Z. Deng, C. Chen, X.-G. Li, and S. P. Ong, ArXiv E-Prints (2019).
[5] C. Chen, W. Ye, Y. Zuo, C. Zheng, and S. P. Ong, ArXiv Prepr. 1 (2018).