数学与系统科学研究院

计算数学所学术报告

报告人：Prof. Stefano de Gironcoli

（ International School for Advanced Studies

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报告题目：

Machine Learning enhancement of Electronic Structure approaches for Crystal Structure Prediction

邀请人：　戴小英 研究员

报告时间：2019 年 4 月 2 日（周二）

上午 10:00-11:00

报告地点：　数学院南楼二层

202 会议室

Abstract:

Machine Learning approaches are gaining much attention in many fields. Crystal Structure Prediction of molecular crystals requires a careful search in a vast potential energy landscape. Methods based on Density Functional Theory, especially if including vdW-aware exchange-correlation functionals, have shown to deliver the desired accuracy [1] but their use come with a significant cost. There is a natural synergy between data-hungry machine learning methods and crystal structure prediction based on ab-initio data. Models that combine Density Functional Theory (DFT) with Machine Learning (ML) promise to deliver the accuracy of DFT at the speed of ML, allowing a more efficient exploration of the structural landscape.

I will briefly introduce the main concepts involved in Machine Learning regression and how this can be integrated with cristal structure prediction tools.I will also introduce a deep neural network training tool, PANNA (Potentials from Artificial Neural Network Architectures), based on TensorFlow framework [2], that is being developed in SISSA by Emine Kucukbenli, Franco Pellegrini, Ruggero Lot and Yusuf Shaidu.

[1] C. Bull et al. "ζ-Glycine: insight into the mechanism of a polymorphic phase transition" IUCrJ 4, p.569 (2017)

[2] M. Abadi et al. "TensorFlow: Large-scale machine learning on heterogeneous systems" (2015)

Introduction of the speaker：

Dr. Stefano de Gironcoli is a professor of Computational Condensed Matter Physics at the International School for Advanced Studies (ISAS)(Scuola Internazionale Superiore di Studi Avanzati (SISSA)). He is a fellow of the American Physical Society since 2009. He is a long time developer and contributor to the open-source Quantum ESPRESSO software distribution. He has made a great contribution to the development of Quantum ESPRESSO, including the optimization of the codes and the methodological developments for accurate and high performance calculations in the framework of density functional theory and their implementation in Quantum ESPRESSO.

His research work also includes the computational physics of condensed matter with contribution to the ab-initio computation of vibrational properties, the physical properties of metallic surfaces and their reactivity toward simple organic adsorbates, and for the structural and mechanical properties of materials of geophysical interest at extreme pressure and temperature conditions.

Professor de Gironcoli has published about 150 research articles in international scientific journals that have been quoted more than 20,000 times in recent literature.

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