



Seminar

Applications of Machine Learning to Materials Modeling

Efthimios Kaxiras

*Department of Physics and School of Engineering and Applied Sciences,
Harvard University*



Time: 4:00pm, Nov. 21, 2017 (Tuesday)

时间: 2017年11月21日 (周二) 下午4:00

Venue: Room W663, Physics building, Peking University

地点: 北京大学物理楼, 西663会议室

Abstract

The last few years have witnessed a surge of activity in machine learning approaches applied to materials science. In this talk I will address both the promise and the limitations of using data science ideas to explore the possibilities of “materials by design”, drawing on examples from recent research in our group. Applications of our work focus on exploring the properties of new materials for energy related problems, including improved batteries, photovoltaics, and new catalysts; in a parallel but distinct type of approach, we have been exploring how machine learning approaches can shed light into fundamental questions like the strength of amorphous solids.

About the speaker

Efthimios Kaxiras is Van Vleck Professor of Pure and Applied Physics, and the Founding Director of the Institute for Applied Computational Science at Harvard University. He was educated at the Massachusetts Institute of Technology where he received a BS in Physics and a PhD in theoretical condensed matter physics. He joined the faculty of Harvard University in 1991 where he currently holds joint appointments in the Department of Physics and in Applied Physics at the School of Engineering and Applied Sciences, and is an Affiliate of the Department of Chemistry and Chemical Biology. He serves on the Editorial Board of several scientific journals, has published over 330 papers in refereed journals and several review articles and chapters in books, as well as a textbook on the structure of solids: “Atomic and electronic structure of solids” .