北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Seminar

ARTIST: Artificial Intelligence for Spectroscopy

Patrick Rinke*

Aalto University

Time: 4: 00 pm, May. 27, 2019 (Monday)

时间：2019年5月27日 （周一）下午4:00

Venue: Room W563, Physics building, Peking University

地点：北京大学物理楼，西563会议室

Abstract

For the study of molecules and materials, conventional theoretical and experimental spectroscopies are well established in the natural sciences, but they are slow and ex- pensive. Our objective is to launch a new era of artificial intelligence (AI) enhanced spectroscopy that learns from the plethora of already available experimental and theoretical spectroscopy data. Once trained, the AI can make predictions of spec- tra instantly and at no further cost. In this new paradigm, AI spectroscopy would complement conventional theoretical and experimental spectroscopy to greatly accel- erate the spectroscopic analysis of materials, make predictions for novel and hitherto uncharacterized materials, and discover entirely new materials.

In this presentation, I will introduce the two AI approaches we have used to learn spectroscopic properties: kernel ridge regression (KRR) and deep neural networks (NN). The models are trained and validated on data generated by density-functional theory calculations for three different molecular data sets: QM9 [1], a well-established small molecule benchmark datasets, a set of amino acid and dipeptide conformers [2] and a set of crystal-forming, optically-active molecules [3]. The molecules are rep- resented by simple, easily attainable numerical descriptors based on nuclear charges and cartesian coordinates [4,5]. The complexity of the molecular descriptor and the diversity of the data sets turn out to be crucial for the learning success, as I will demonstrate for KRR [6]. I will then show, how we can learn spectra (i.e. continuous target quantities) with NNs. We design and test three different NN architectures: multilayer perceptron (MLP), convolutional neural network (CNN) and deep tensor neural network (DTNN). Already the MLP is able to learn spectra, but the learn- ing quality improves significantly for the CNN and reaches its best performance for the DTNN [7]. Both CNN and DTNN capture even small nuances in the spectral shape. In a showcase application of this method, the structures of 10k previously unseen organic molecules are scanned and instant spectra predictions are obtained to identify molecules for potential applications [7].

∗ This work was performed in collaboration with A. Stuke, K. Ghosh, L. Himanen, M. Rupp, C. Kunkel, P. B. Jørgensen, M. N. Schmidt, M. Todorović, and A. Vehtari

[1] R. Ramakrishnan, P. O. Dral, M. Rupp, and A. von Lilienfeld, Sci. Data 1, 140022 (2014)
[2] M. Ropo, M. Schneider, C. Baldauf, and V. Blum, Sci. Data 3 (2016)
[3] C. Schober, K. Reuter, and H. Oberhofer, J. Phys. Chem. Lett. 7, 3973 (2016)
[4] M. Rupp et al. Phys. Rev. Lett. 108, 058301 (2012)
[5] H. Huo and M. Rupp, arXiv:1704.06439
[6] A. Stuke, M. Todorović, C. Kunkel, M. Rupp, K. Ghosh, L. Himanen, and P. Rinke, arXiv:1812.08576
[7] K. Ghosh, A. Stuke, M. Todorović, P. B. Jørgensen, M. N. Schmidt, A. Vehtari and P. Rinke, Adv. Sci. 6, 1801367 (2019)

About the speaker

Patrick Rinke is a professor in Helsinki, Finland, at Aalto University's Department of Applied Physics. He obtained his PhD from the University of York, England, and then did post-doctoral stays at the Fritz Haber Institute of the Max Planck Society in Berlin, Germany, and the University of California at Santa Barbara, USA, before joining Aalto University. His research group develops electronic structure and machine learning methods and applies them to pertinent problems in physics, chemistry and materials science. Recent highlights include the application of the GW Green's function approach to core excitations, a dynamical configuration interaction approach for treating strongly correlated molecules, artificial intelligence for spectroscopy and active learning smart data approaches for optimization. Aside from science, he likes cats and green tea.