Aalto University

Dissertation press release 3.8.2020

Using machine learning to accelerate the design of future electronic materials – how machine learning algorithms can be used to enhance lab experiments

Title of the dissertation	Machine learning for spectroscopic properties of organic molecules
Contents of the dissertation	Conventionally, in order to tailor materials that meet market demands, materials engineers study substances at the molecular level using techniques such as electron microscopy. This way, they can visualize single molecules and atoms within a substance, alter their properties or create entirely new molecules by rearranging the atomic order. Properties of interest are, for instance, the orbital energies of a molecule. The difference between the highest and lowest orbital energy translates to the amount of energy that a molecule can store. This is important to know in order to find better materials for solar cells, fibers or computer chips. To improve, for example, the device performance of OLEDs (organic light emitting diodes), which are progressively adopted as a standard display technology for TV and phone screens, new organic materials need to be created that can store a specific amount of energy. However, the market need for new materials is growing at a rate that outpaces laborious experimental design techniques. Likewise, computational tools that simulate materials properties based on quantum mechanics are too expensive to be run on a large scale. To tackle this problem, machine learning (ML) – a branch of artificial intelligence (AI) that creates computer systems which automatically and progressively learn from data and improve through experience – can be combined with materials science technologies. In my dissertation, I develop an AI system that efficiently analyzes existing materials data of organic molecules and gradually learns from it. After training, my AI system is able to predict orbital energies of new molecules for which no data are yet available. Based on these predictions, materials engineers can pick a new molecule that might be suitable for OLED applications, before this molecule is even fabricated. My ML model may act as an expert materials recommendation system alongside experimentation, by suggesting specific types of molecules that should be made and tested, thus efficiently assisting in designing suitable OLED materials.
Field of the dissertation	Applied Physics, Computational Electronic Structure Theory
Doctoral candidate	Annika Stuke, MSc
Time of the defence	14.08.2020 at 16:00
Place of the defence	Public defence will be organized via Zoom: https://aalto.zoom.us/j/68194827869
Opponent	Professor Rampi Ramprasad, Georgia Institute of Technology, USA
Custos	Professor Patrick Rinke, Aalto University School of Science, Department of Applied Physics
Electronic dissertation	http://urn.fi/URN:ISBN:978-952-60-3967-1
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