Machine learning accelerated electronic transport calculations for complex materials

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Hello, my name is Phytos Neophytou and I'm a professor in the School of Engineering at the University of Warwick and this is the presentation for the HetSys CDT project entitled Machine Learning Accelerated Electronic Transport Calculations for Complex Materials. So I'll give you a brief overview of what this project is about. Over the last couple of decades, materials chemistry has come up with the capabilities to synthesize a plethora of new materials and their alloys.

These materials are complex in nature, they have complex unit cells and they don't have energy surfaces like the normal spherical ones we're used to for simple materials like silicon for example, but they have energy surfaces like the ones we see here to the left of the screen with elongated features, many valleys and tubes and this complexity, although it's difficult to deal with computational point of view, it's actually what drives the enhanced properties that we are looking for in our new technologies. Now when we try to evaluate the electronic properties, we typically have a DFT calculations that give us the electronic structure and the energy surfaces and then we go through a very computationally intensive process in extracting what we call the scattering rates. This scattering rate is a very complex object, it's with many dependencies and many different details that need to be captured and takes enormous computational time in the supercomputers that we are using.

But once we have that, then you use the Boltzmann transport equation and there's software for that one that gives you the electronic transport properties like the conductivity, the mobility or the zebra coefficient of the materials. Now the project bypasses that very expensive computational beat by creating a highly efficient machine learning algorithm that actually connects you all the way from the electronic structures to the Boltzmann transport equation and electronic properties and that one will hopefully accelerate and allow the electronic transport calculations for hundreds, maybe thousands of materials that are out there without going through this hugely expensive process of scattering rates. Of course those methodologies that give you the scattering rates will be used and we have codes for that one in order to develop test sets of this machine learning in order to train our machine learning algorithm.

But finally what we want to do is to bypass it and be able to advance this field of electronic materials with complex structures based on machine learning methods that would allow the exploration of a large space of materials. Thank you very much.