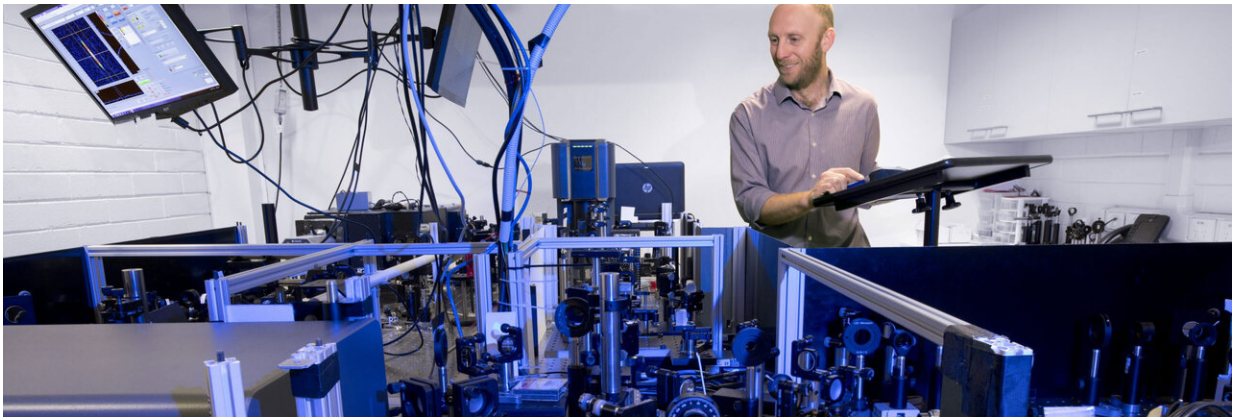


Teaching a machine how to identify imperfections in 2-D materials

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Credit: FLEET

Just as James Cameron's Terminator-800 was able to discriminate between "clothes, boots, and a motorcycle," machine-learning could identify different areas of interest on 2-D materials.

The simple, automated optical identification of fundamentally different physical areas on these materials (eg, areas displaying doping, strain, and electronic disorder) could significantly accelerate the science of atomically [thin materials](#).

Atomically thin (or 2-D) layers of matter are a new, emerging class of materials that will serve as the basis for next-generation energy-efficient

computing, optoelectronics and future smart-phones.

"Without any supervision, machine-learning algorithms were able to discriminate between differently perturbed areas on a 2-D semiconducting material," explains lead author Dr. Pavel Kolesnichenko. "This can lead to fast, machine-aided characterization of 2-D materials in the future, accelerating application of these materials in next-generation low-energy smart-phones."

Automation opening up the field of atomically thin materials

After the 2004 success of a single layer of pencil's graphite (graphene) as a wonder semi-metallic material with many peculiar properties, scientists around the world realized that other layered materials can also be thinned down to a single layer (a 'monolayer').

Since then, dozens of other monolayers have been obtained, including metals, semiconductors, insulators, and more-exotic quantum materials such as topological-insulators, superconductors and ferromagnets.

Having this monolayer-zoo at their disposal, materials scientists have used them like "LEGO"-blocks: for example stacking them in many different combinations to construct next-generation transistors, batteries, memory cells and photodiodes.

All these devices, however, have been assembled manually and exist as one-off prototypes. There is still a long way towards their industrial-scale production and commercialisation.

Several factors contribute to the hindrance of the progress. First is the lack of full control over the fabrication of monolayer materials. In

addition, current characterisation techniques are complicated and require the eye of an experienced researcher. Finally, due to the extreme thinness of the materials, the latter are extremely sensitive to various perturbations, many of which are introduced unintentionally.

Understanding these perturbations is a non-trivial task, as they can have a combined effect and have to be disentangled.

Dr. Pavel Kolesnichenko and Prof Jeffrey Davis (Swinburne University of Technology) realized that the ungrateful task of characterization of 2-D materials could be accomplished by machines in a rapid and automated manner.

"In order to understand the impact of different perturbations and minimize or control their presence, it is important to be able to identify them and their spatial distribution rapidly and reliably," said Prof Davis, who is a chief investigator in ARC Centre of Excellence in Future Low-Energy Electronics Technologies (FLEET).

Working with FLEET colleague Prof Michael Fuhrer (Monash University), they applied unsupervised [machine-learning](#) algorithms to characterize the semiconducting monolayer of tungsten disulphide. The data was acquired by simple apparatus involving a microscope and a spectrometer. The learning algorithms then were able to discriminate between the areas on a monolayer flake affected by doping, strain, disorder, and the presence of additional layers.

This is the first time such a systematic disentanglement of these perturbations has been performed.

The task was accomplished by embedding the acquired data into an artificially constructed multi-dimensional parameter space. Learning algorithms were then allowed to find a way to visualize the data in comprehensible two dimensions and in the most representative way,

where each perturbation formed its own data-cluster.

The team built on previous scientific results in the field including their previous publication, where they disentangled perturbations using correlated photoluminescence and absorption spectra.

"So many factors can affect optoelectronic properties of 2-D materials, including the type of substrate, additional doping, strain, the presence of wrinkles, defects, and environmental molecules—you name it," said Dr. Pavel Kolesnichenko (now a postdoc at Lund University). "Thus, moving to a multi-dimensional parametric space seemed to be a natural next step."

"We also hope the research will motivate scientists to apply similar ideas to other 2-D materials and using other imaging modalities," says Pavel.

In the era of data-driven science and technology, the authors hope that their research will motivate the creation of a large labeled dataset, where labels (such as 'doping,' 'strain,' etc) would be assigned by experienced researchers. This dataset would be then used to train deep neural networks to characterize 2-D materials in a fraction of a second. The researchers believe that their work will help to introduce standards for characterisation of monolayer matter, approaching the moment of large-scale use of low-energy smart-phones and computers in the future.

More information: Pavel V Kolesnichenko et al. Multidimensional analysis of excitonic spectra of monolayers of tungsten disulphide: toward computer-aided identification of structural and environmental perturbations of 2-D materials, *Machine Learning: Science and Technology* (2021). [DOI: 10.1088/2632-2153/abd87c](https://doi.org/10.1088/2632-2153/abd87c)

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(2019). [DOI: 10.1088/2053-1583/ab626a](https://doi.org/10.1088/2053-1583/ab626a)

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