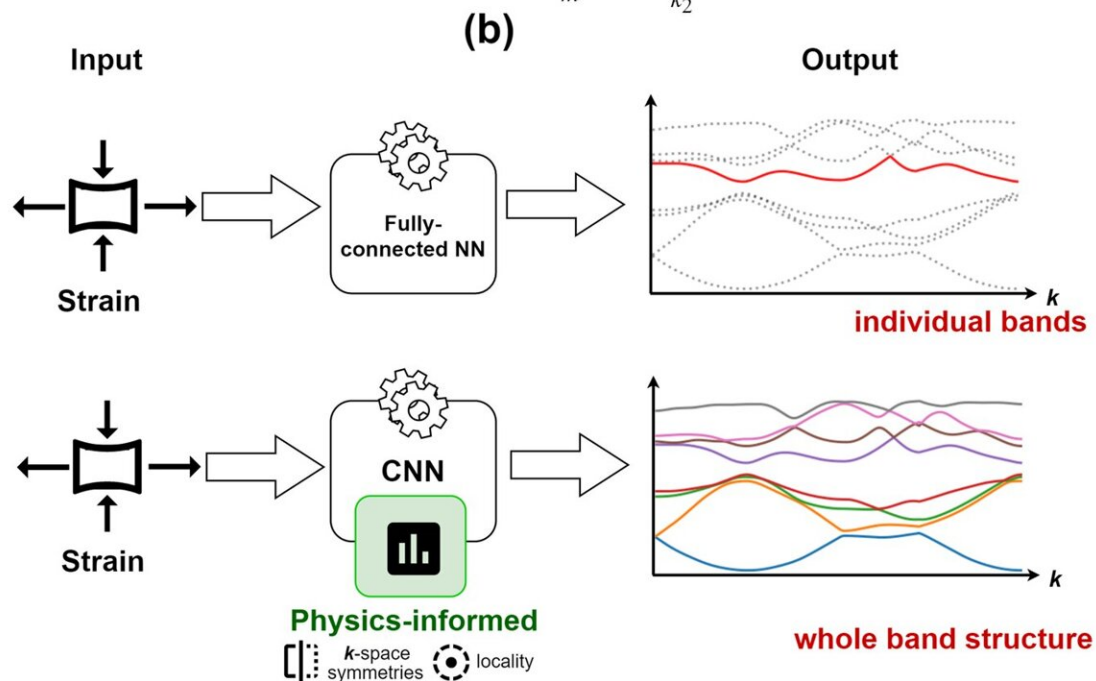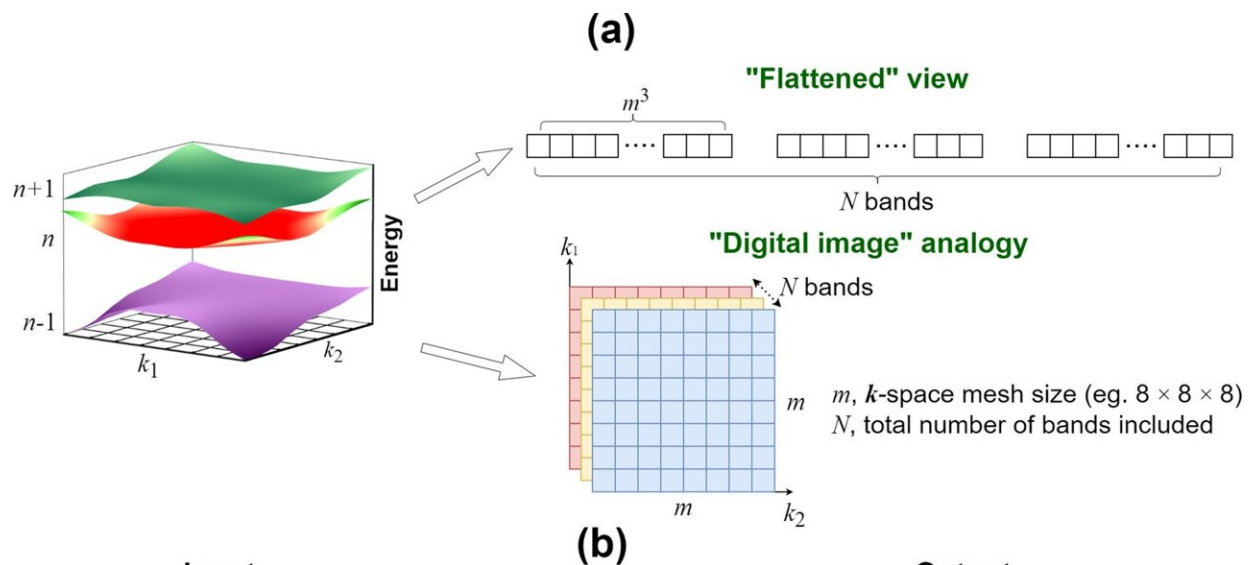# Putting a strain on semiconductors for next-gen chips

July 14 2021

a Different representation of a band structure. In the "flattened" view, a band structure is represented as N stacked flattened arrays (vectors) and processed like independent values. Each array is m3 in length. In the "digital image" analogy, the band structure is envisioned as N different 3D images stacked together, each of which has a "voxel" dimension of m × m × m. The eigenvalues on an energy band can then be thought of as the "color-scale" of the voxels. b Comparison of the two different approaches to ML. We predict the eigenvalues for each energy band separately by utilizing the "flattened" band structure representation to obtain the entire band structure. Credit: DOI: 10.1038/s41524-021-00538-0

Skoltech researchers and their colleagues from the U.S. and Singapore have created a neural network that can help tweak semiconductor crystals in a controlled fashion to achieve superior properties for electronics. This enables a new direction of development of next-generation chips and solar cells by exploiting a controllable deformation that may change the properties of a material on the fly. The paper was published in the journal *npj Computational Materials*.

Materials at the nanoscale can withstand major deformation. In what's called the strained state, they can exhibit remarkable optical, thermal, electronic, and other properties due to a change in interatomic distances. The intrinsic properties of a strained material may change, with the semiconducting silicon, for instance, transforming into a material that conducts the electric current freely.

Moreover, by varying the strain level, one can change these properties on demand. That notion has given rise to an entire field of inquiry: elastic strain engineering, or ESE. The approach can be used, for example, to modify the performance of semiconductors, providing a potential workaround for the impending Moore's law limit, when we exhaust our other options for increasing chip performance. Another possible application lies within the field of solar cell development. As study co-

author Alexander Shapeev from Skoltech explains, one can design a solar cell with tunable properties that can be changed on demand in order to maximize performance and adapt to external circumstances.

In their [previous work](#), Skoltech Ph.D. graduate Evgenii Tsymbalov, Associate Professor Alexander Shapeev, and their colleagues used ESE to turn nanoscale diamond needles from insulating to highly conductive and metal-like, providing an insight into the range of possibilities with this technology. Now, the team has introduced a convolutional [neural network](#) architecture that can guide ESE efforts for semiconductors.

"The neural network we have designed takes the strain tensor as an input and predicts the electronic band structure—a physical 'snapshot' that describes the electronic properties of a strained material. It may then be used to calculate any properties of interest, including the bandgap, its properties, and electron effective mass tensor," Shapeev said.

This work continues prior research and expands on it. "We go beyond the previously used approaches by designing and implementing a tailored model based on the convolutional neural network architecture, for the ESE task," Tsymbalov said. "We also take the [physical properties](#) and symmetries into account in order to improve the model."

The approach combines various data sources, for example, the computationally cheap yet inaccurate with the precise but expensive ones in order to boost the accuracy and convergence of the model. "Another distinct feature is active learning—we allow the model to guess what data may be the most useful to obtain in the next training stage, and use it for training. In the final stage, the network is trained on a set of computationally expensive data from the very accurate GW-based calculations, and this procedure allows us to reduce the amount of computations needed," Tsymbalov added.

The team notes that its new neural network is "more versatile, accurate, and efficient in its capacity to facilitate autonomous deep learning of the electronic band structure of crystalline solids" than state-of-the-art solutions. This makes it faster and more accurate at search and optimization within the strain space, which leads to the optimal strain values for given figures of merit.

In their earlier work, the researchers tested a previous iteration of the model in the scenario of a repeating in situ experiment on diamond. "Alas, for now there is no device that can deform the diamond with an arbitrary 6D deformation tensor, yet there are teams and labs pursuing this direction from the experimental point of view," Tsymbalov commented.

This study is part of a yearslong collaboration between Skoltech, the Massachusetts Institute of Technology, and Nanyang Technological University, with the Skoltech scientists focused on the computational and machine learning aspect and their colleagues in charge of the physical component of the work. "We are currently working on our next paper, which is devoted to the boundaries of admissible elastic strains. It is an important topic since the theoretical limits of safe elastic deformation for ESE are yet to be discovered," the researcher concluded.