Elastic strain engineering meets active learning: the case of semiconductors

Evgenii Tsymbalov[1], Zhe Shi[2], Alexander Shapeev[1], Ju Li[2]

[1]Skolkovo Institute of Science and Technology, [2]Massachusetts Institute of Technology

Elastic strain engineering opens new opportunities for the optimization of magnetic, electrical, and optical characteristics of nanostructured materials: fundamentally, the electronic structure of a crystal changes with the elastic strain. To map out the whole room available for the strain engineering of silicon, germanium, diamond (carbon) and other materials, an understanding of the band topology changes in the six-dimensional strain space is imperative, and exhaustively exploring the band structure by the traditional theory is rather formidable. Surrogate models based on machine learning modules can efficiently represent the dependence of the most technologically relevant electronic properties of silicon on the strain. In our work, we demonstrate that these models, relying on a limited amount of data from first-principles calculations, may reproduce the required properties with sufficient accuracy. The data amount needed for the training may be further reduced using the active learning techniques, leading to the rapid development of surrogate models for material engineering.