Understanding Materials Structure by Using Machine Learning

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Clarifying the nature of materials is one of the main roles of materials science [1]. Traditionally, this process has been performed by experimental or quantum computational approaches [2]. However, these approaches have significant limitations on the time scale, the computational cost, and require high-quality equipment [3]. Recently, data-driven approach with the use of advanced machine learning techniques is expected to overcome those limitations and therefore speed up the process of knowledge discovery in materials science [4].

In this paper, we propose a machine learning method to extract meaningful and useful knowledge about the structure and physical properties of materials from data. We fragment structures of materials into smaller element parts, called "local structures", and then investigate the contributions of these parts to the target properties using linear models. The obtained results demonstrated that our method can learn the atomization energy of molecular systems, the formation energy of the solid magnetic system with an accuracy of the chemical precision level. Further, we can extract the knowledge related to local structures, such as the associated energy of local structures, the map between geometry structure and atomic energy, and the similarity between elements in term of the contribution to physical properties of materials. The great ability of prediction and knowledge extraction leads our method to have the potential to accelerate the process of designing and discovering new advanced materials.

Reference:

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