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Machine learning in materials science

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Abstract

Abstract Traditional methods of discovering new materials, such as the empirical trial and error method and the density functional theory (DFT)based method, are unable to keep pace with the development of materials science today due to their long development cycles, low efficiency, and high costs. Accordingly, due to its low computational cost and short development cycle, machine learning is coupled with powerful data processing and high prediction performance and is being widely used in material detection, material analysis, and material design. In this article, we discuss the basic operational procedures in analyzing material properties via machine learning, summarize recent applications of machine learning algorithms to several mature fields in materials science, and discuss the improvements that are required for wideranging application.

Keywords: machine learning, materials discovery, materials design, materials property prediction, density func

Full text

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