Machine learning for computational materials physics

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In the rapidly developing field of AI for Science, especially in computational materials physics, AI has attracted significant attention as a driving force for understanding the physical structure-property relationships and accelerating the discovery of new materials. In this talk, I will review recent advances, challenges, and opportunities of AI in the field of computational materials science.

I will begin my talk by discussing the early stage of developing feature engineering techniques used in predicting physical properties directly from material structures[1]. The development of a materials database represents the middle stage, enriching large quantities of material data as the foundation for training AI models[2]. Finally, I will introduce the concept of physics-integrated deep learning models. By incorporating fundamental physical principles into the architecture of deep learning algorithms, one can enhance the models' predictive power and interpretability[3]. This approach not only improves the accuracy of our predictions but also ensures that the models adhere to the laws of physics.

References

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