

From Schrödinger equation to large atomic model

This report briefly reviews the historical development of atomic models, from John Dalton's atomic theory to the establishment of quantum mechanics, and discusses the challenges faced by modern atomic simulation methods. The report highlights the application of machine learning models in atomic-scale simulations, particularly the Deep Potential Molecular Dynamics (DeePMD) model, which offers both accuracy and efficiency in handling large-scale atomic systems. Additionally, the limitations of existing machine learning models are discussed. To overcome these limitations, the report reviews several attempts to develop more general-purpose machine learning models and points out the difficulties in creating a universal model that spans multiple domains and tasks. Finally, the report proposes preliminary attempts to establish the Large Atomic Model (LAM), specifically DPA-2, detailing its model architecture and the pre-training, fine-tuning, and knowledge distillation workflow. The report introduces the OpenLAM initiative, an open-source project aimed at advancing the development of large atomic models.