

AI for material science: from data-driven to interpretable models of physical systems

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In this talk, we will explore the potential of AI in material science, focusing on data-driven and interpretable models of physical systems for 2D materials with defects. The presentation will cover various AI techniques, such as graph neural networks and autoencoders, and their applications in predicting material properties, generative design, and inverse design problems. Additionally, challenges such as the high cost of cutting-edge AI models, limited and diverse datasets, and interpretability in the context of physical systems will be discussed alongside ethical considerations related to the application of AI in material science.