PiAI Seminar Series: Physics informed AI in Plasma Science
9:00-10:00, 17 June 2024 (EDT)
15:00-16:00, 17 June 2024 (CEST)
22:00-23:00, 17 June 2024 (JST)
Web Seminar

Machine Learning Enabled Prediction of Nanoparticle Growth in Nonthermal Plasmas: Bridging the Gap Between Atomistic and Continuum Scales

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Understanding the properties of materials generated in nonthermal plasmas (NTPs) is crucial for tailoring their synthesis for specific applications. However, modeling the transition from gas phase to solid phase remains a challenge, particularly due to the nonequilibrium nature of NTPs. In this work, we focus on silane nanoparticles (NPs) as a case study to explore the challenges of atomistic simulations under these conditions and how machine learning (ML) can be leveraged to achieve generalization and reduce computational costs.

We examine the most complex scenario where colliding species deviate from thermal equilibrium. We investigate how different ML models and molecular representations affect prediction accuracy and emphasize the importance of selecting an appropriate representation, especially for generalizing beyond the training data's chemical space. We continue showing progress toward building interpretable representations for small molecules and nanoparticles to predict their thermodynamic properties, even though capturing reactivity remains an ongoing challenge.

We conclude by discussing more efficient approaches that are applicable when less general forms of nonequilibrium can be assumed and how ML models can be combined to estimate kinetic rate constants for reactions involving small and larger species.