PiAI Seminar Series: Physics informed AI in Plasma Science
8:00-9:00, 15 April 2024 (EDT)
14:00-15:00, 15 April 2024 (CEST)
21:00-22:00, 15 April 2024 (JST)
Web Seminar

Machine Learning Boosted Design of Plasma-Enhanced Catalytic Ammonia Cracking

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Abstract

Hydrogen (H_2) is an energy carrier with high energy content (142 kJ/g) and a non-polluting energy source. Hydrogen's implementation is hindered, however, by delivery and storage issues. Ammonia (NH_3) is being studied as a storage medium for H_2 due to its high H_2 density, ability to easily condense, storage and distribution. However, thermal NH_3 cracking to generate H_2 usually requires the reaction temperatures above 773 K and an earth-rare metal catalyst (i.e., Ru) to achieve complete conversion. One strategy to activate ammonia at mild conditions over earth-abundant metal catalysts is by applying non-thermal plasma since the vibrationally excited species produced in non-thermal plasmas lower the temperature of NH_3 cracking. However, modelling interfacial plasma-surface interaction is a multi-scale problem and building such simulation for a complex reaction mechanism over a large search space of catalyst materials is computational immense.

To solve the above challenge, it is important to identify the key descriptor that impacts the overall rates of ammonia cracking under non-thermal plasma conditions and apply such descriptor to screen the large search space of catalysts. Thus, we first built the microkinetic model and machine learning algorithm for ammonia cracking. AI-predicted catalysts will be further validated by experiments. The integration of multi-scale modeling, machine learning algorithms and experiments will facilitate materials development in interfacial plasma-surface reaction rather than trial-and-error.