Opening for a Postdoctoral Fellowship in ML Models for Catalyst Degradation

SUMMARY: A Postdoctoral position is available for immediate start in catalysis data science. We are seeking a highly qualified candidate with a detailed understanding of heterogeneous catalysis as well as extensive experience with machine learning. Experience with theoretical/computational catalysis is also desirable.

KEYWORDS: Catalysis data science, machine learning

DESCRIPTION: The goal of the project is to develop machine learning models to predict the degradation/sintering of nanoparticle catalysts for the reverse water gas shift reaction, by combining experimental and computational training and target data. The project involves the development of active learning ML frameworks to drive the selection of experiments and simulations. The initial focus will be on the small data regime with high consideration to model uncertainty, feature selection and model interpretability. The project is highly collaborative and includes research groups at several US national labs and universities. The research is funded through US Department of Energy through the Accelerate Innovations grant. The position is initially for 1 year, with the possibility of continuation based on a yearly evaluation.

A successful candidate will satisfy the following:

- A PhD in chemical engineering, materials science, physics, chemistry, or related field
- A strong understanding of thermal heterogeneous catalysis, preferably with experience in computational modeling.
- Machine learning experience as well as a strong proficiency in Python programming and data analysis.
- Excellent communication skills and a career level-appropriate publication track record.
- The ability to work independently and collaboratively in a diverse research team.

Preview of applications begins immediately. Applications are accepted until the position is filled. Please include a letter of motivation, C.V. with list of publications, coding contributions (such as git repository), and the contact information for two to three academic references.

CONTACTS: Please send application to Kirsten Winther (winther@stanford.edu) or contact for further details on the position.