

DEPARTMENT OF CHEMISTRY

## Connecting data and physical models with embedded machine learning at electrochemical interfaces and beyond

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As data-driven methods become more prominent throughout science, we need new ways of combining physical understanding with data from experiments and first principles calculations. This talk will present a unique paradigm for combining physical models and data-driven elements, in which embedded data-driven functions represent well-defined physical quantities, subject to independent measurement and calculation. A fast-evaluating, decomposable Gaussian process is an enabling development. Examples to be discussed include learning inhomogeneous free energy functions at ionically charged surfaces and interfaces from electron and scanning probe microscope data.



Students, meet the speaker before the seminar in a student/postdoc session from 3:00 - 3:20 pm

Date: Time: Location: Clark Hall 112

Wed. February 28, 2024 3:30-4:30 pm