



# DEPARTMENT OF PHYSICS AND ASTRONOMY

## COLLOQUIUM *IN-PERSON EVENT*



Machine learning aided Hamiltonian extraction and inverse modeling of materials

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A Hamiltonian describes the interactions among constituent atoms and gives the total energy of a physical system. If a material's Hamiltonian is known, forward simulations such as molecular dynamics and Monte Carlo simulations can be carried out to study the thermodynamics of the material. However, fitting Hamiltonian model parameters from experimental measurements is often a challenging inverse problem. In this talk, I will highlight our team's current efforts in developing novel methodologies for constructing Hamiltonians from experiments. Emphasis will be placed on two concrete examples: fitting model Hamiltonian for spin ice compound  $\text{Dy}_2\text{Ti}_2\text{O}_7$  from neutron scattering data, as well as training neural network interatomic potentials to first principles calculations.



**Thursday, October 19, at 3:55 PM**

***IN-PERSON EVENT ROOM 202***

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