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Extract microscopic information of materials from Neutron Scattering data using a Machine Learning assisted approach.

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Precise modeling of a material is a key to understand its underlying interactions and physics but also revealing the competing phases in the nearby interaction space. Highly frustrated systems are important due to the richness in physics and diversity of phases including spin liquids with exotic topological states they display. Here, we present a machine learning workflow to fit multi-experimental data sets to find an optimal Hamiltonian while undertaking phase classification and extracting information about the topography around the region of interest. Experimental data from a spin-ice material, $\text{Dy}_2\text{Ti}_2\text{O}_7$ including diffuse neutron scattering, heat capacity and susceptibility are utilized. This approach is shown to provide the best model in an efficient and effective way but also is powerful at planning the best experimental strategies.

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