Contribution ID: **313** Type: **Talk**

【711】Determination of skyrmion-hosting transition metal-oxide Hamiltonian with predictive guidance from ab-initio quantum chemistry

Tuesday 10 September 2024 16:30 (30 minutes)

The remarkable tunability and inherent functionality of many quantum materials stem from intricate many-body states in which several degrees of freedom are entangled. These microscopic complexities manifest in collective excitations, forming the basis of their distinct properties. Inelastic neutron scattering is pivotal in testing theoretical predictions to unravel emergent quantum effects. However, in many cases it is challenging to find appropriate microscopic Hamiltonian candidates that can be refined against experimental observations. In this talk I will show that ab-initio quantum chemistry is a promising tool that can guide us in determining the microscopic interactions in transition metal-oxides.

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Session Classification: Neutron Science

Track Classification: Neutron Science