

INVITATION

Department of Condensed Matter Physics

Is pleased to invite you to the lecture

Computing and understanding magnetic exchange with
quantum chemistry

by

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Date: 12 November 2025

Time: 11:00

Venue: Lecture room F1, Building 6, Faculty of Science, Kotlářská 2, Brno

Accurately predicting magnetic interactions requires methods that reliably capture spin-state energetics and electronic correlation. This talk presents wavefunction-based quantum chemistry approaches for computing exchange couplings, discusses the mapping of ab initio results to effective model Hamiltonians, and illustrates applications to transition metal compounds with strong spin-orbit coupling.

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