Contribution ID: **31** Type: **Invited Oral**

Computational chemistry - scientific results and state-of the art software tools

Wednesday, 4 June 2025 09:30 (30 minutes)

The analysis of neutron data in the context of magnetic structure relies heavily on the fitting of the parameters of an effective Hamiltonian model. The complexity of the systems under study leads to the increase of the number of parameters of these models and a good starting guess for the fit becomes crucial. Ab initio calculations on these systems can provide quantitative estimate for the number of parameters to consider and for their values. In this talk I will show our recent developments in the context of the calculation of magnetic excitations from ab initio methods and put it in the more general framework of the role of simulations in the analysis of neutron data in the ILL and the development of an integrated data platform (C-Lab) for the neutron users.

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