Contribution ID: **2** Type: **not specified**

Revisiting μSR results in MnO

Thursday, 5 September 2024 11:00 (25 minutes)

MnO has been the skeleton in the closet for the numerous scientists that have been trying to model and understand the μSR results of magnetic oxides [1-8]. In zero field, this material shows a single precession frequency whose origin was hard to reconcile with the proposed muon sites and the possible formation of muonium-like states [4-6]. The picture is further complicated by a time-window dependent Knight shift discovered by Uemura and co-workes [3], where different Knight shifts are obtained considering the asymmetry in the first μs as compared to that for the second μs, etc. The puzzle is eventually solved by highlighting the role of symmetry, magnetostriction, and muon diffusion in the system. In this talk I will describe how first principles simulations and molecular dynamics exploiting machine learning force fields allow to verify or disprove various proposals that have been discussed over the years [3-8] on the microscopic description of the muon life in MnO. This finally allows to easily explain both the zero-field data and the unusual time-dependent Knight shift in MnO, solving, possibly for the second time [9], an old puzzle.

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Session Classification: Science Session

Track Classification: Computational