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Revisiting μ SR results in MnO

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MnO has been the skeleton in the closet for the numerous scientists that have been trying to model and understand the μ SR 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-workers [3], where different Knight shifts are obtained considering the asymmetry in the first μ s as compared to that for the second μ s, 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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