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Pressure Effect on Hydrogen Tunneling and Vibrational Spectrum in α-Mn ALEXANDER KOLESNIKOV, ANDREY PODLESNYAK, Oak Ridge National Lab, RAVIL SADYKOV, VLADIMIR ANTONOV, MICHAIL KUZOVNIKOV, RAS, Moscow , GEORG EHLERS, GARRETT GRANROTH, Oak Ridge National Lab — The pressure effect on the tunneling mode and vibrational spectra of hydrogen in α-$MnH_{0.07}$ has been studied by inelastic neutron scattering. Applying hydrostatic pressure of up to 30 kbar is shown to shift both the hydrogen optical modes and the tunneling peak to higher energies. First-principles calculations show that the potential for hydrogen in α-Mn becomes overall steeper with increasing pressure. At the same time, the barrier height and its extent in the direction of tunneling decrease and the calculations predict significant changes of the dynamics of hydrogen in α-Mn at 100 kbar, when the estimated tunneling splitting of the hydrogen ground state exceeds the barrier height. Acknowledgments: Research at ORNL SNS was supported by the Sci. User Facilities Division, Office BES, US DOE, and was sponsored by the LDRD Program of ORNL, managed by UT-Battelle, LLC, for the US DOE. It used resources of the Nat. Energy Res. Sci. Comp. Center, which is supported by the Office of Sci. US DOE under Contract No. DE-AC02-05CH11231. A support by a Grant of the Program on Elementary Particle Physics, Fundamental Nuclear Physics and Nuclear Techn. RAS is also acknowledged.

Alexander Kolesnikov
Oak Ridge National Lab

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