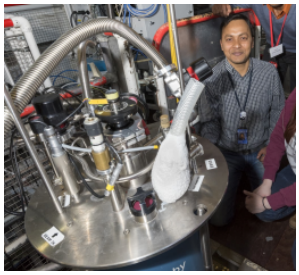

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Quantum tunnelling between muon sites in methylated benzene crystals

Monday, 11 September 2023 17:50 (10 minutes)

We present simulations of the effect of quantum tunnelling between muonium sites in benzene crystals that contain methyl groups. These are added to different carbon atoms, such that they alter the available transition pathways for tunnelling between candidate muon sites. The calculations are based on density functional theory, combining phonon computations (of the zero point energy of the muon) and transition state computations (of the height of the potential barrier between sites) in order to estimate the transition rates between sites and so determine which site pairs the muon can tunnel between during its lifetime. Our results are then used to simulate avoided level crossing (ALC) spectra, allowing us to assess the effectiveness of this methodology.

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