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Theory complements β-NMR studies: correlation time of 23Na+ in liquids

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The molecular environment around different ions in liquids and solids can be determined experimentally using the technique of β-NMR, based for example on the relaxation time T1. However, to interpret T1 correctly in liquids, one needs to take into account the underlying dynamics, which can be done by combining β-NMR results with calculations of the molecular correlation times. Several theoretical methods can be used, such as molecular dynamic (MD), density functional theory (DFT), or a combination of quantum mechanics with molecular mechanics (QM/MM).
To complement β-NMR studies on short-lived 26Na in different ionic liquid hosts, in the present work MD simulations have been applied to study the dynamics of water molecules around the Na+ ion (using the Amber software), before the application in ionic liquids. The obtained correlation time value is in good agreement with other computational results. This method can be now applied to other environments, like ionic liquids.
The poster will present the theoretical approach, the obtained results compared to literature values, and will present them in the context of β-NMR studies performed at ISOLDE.

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Density Functional Theory study of Cd impurities in Molybdenum Trioxide

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Transition metal oxides semiconductors (TMOs) are known for their special optical and electrical properties with wide-ranging applications, including gas sensing, storage devices such as Li-ion batteries, solar cells, and catalysts[1,2]. Among different types of TMOs, there is a class of materials that are distinguished by their unique layered structure and multiple oxidation states, such as MoO_3, WO_3, and V_2O_5. The molybdenum trioxide (MoO_3) is known for its photo-, thermo- and electrochromism, high catalytic activity[3]. The MoO_3 has found in different structural phases including the orthorhombic phase, α-MoO_3; monoclinic phase, β-MoO_3; metastable phase at high-pressure conditions, β′-MoO_3; and hexagonal phase, h-MoO_3[4]. Among them, the α-MoO_3 is the most stable

crystal phase and it has a layered structure consisting of van der Waals bonded sheets of distorted edge-sharing Mo–O_6 octahedra in which Mo atoms are bounded by three distinct types of oxygen atoms[5].

In this research, the structural properties and hyperfine parameters of ^{111m}Cd(^{111}Cd) impurities in α-MoO_3 are investigated by first-principle calculations in the framework of density functional theory (DFT). The Perdew–Burke–Ernzerh of generalized gradient approximation (GGA-PBE), and GGA-PBE plus Hubbard-U corrections for onsite Coulomb interactions are used in the DFT calculations. In the calculations performed, the effect of van der Waals forces between layers is employed using the DFT-D3 method[6]. To interpret the experimental results, different configurations around the Cd atom including the different types of oxygen vacancies are simulated. The comparison of experimental data with calculated hyperfine parameters indicates that the Cd atom is predominantly located in the interstitial lattice site of MoO_3, and also the oxygen vacancy is most likely to form on the 2-fold coordinated (O_2) atoms.

The results of this work demonstrate the benefit of first-principle calculations for solving the outstanding questions arising from the experiment.

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Production and purification of 129m,131m,133mXe for a new medical imagine technique, gamma-MRI

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The gamma-MRI is a novel imaging modality that should allow the simultaneous exploitation of the sensitivity of gamma detection (SPECT) and the spatial resolution and flexibility of MRI. The approach uses highly-polarized gamma-emitting nuclei, which exhibit anisotropic gamma-ray emission that will be used for signal detection – decrease in the number of gamma rays emitted longitudinally to the spin (and magnetic field). The first nuclei used in the project will be $11/2^-$ spin ^{129m}Xe ($T_{1/2}$=8.88 days), ^{131m}Xe ($T_{1/2}$=11.84 days) and ,^{133m}Xe ($T_{1/2}$= 12.19days).

The efficient production and purification of the ^{129m,131m,133m}Xe is one of the first milestones in the gamma-MRI project. This poster will concentrate of two main methods of production tested so far: neutron irradiation of enriched stable ^{128}Xe (product: ^{129m}Xe) and ^{130}Xe (product: ^{131m}Xe) at the ILL reactor in Grenoble, and collection of ^{129m,131m,133m}Xe in gold foils at GLM chamber