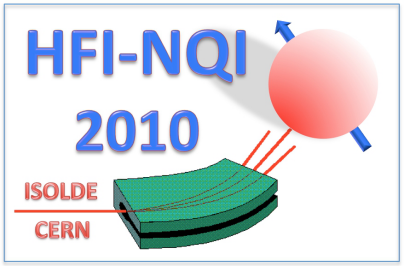

Contribution ID: **88** Type: **POSTER**

The nuclear quadrupole moment of the 245 keV excited state of 111Cd

Several nuclear experimental techniques including nuclear magnetic resonance, nuclear quadrupolar resonance (NQR), time-differential perturbed-angular correlation (TDPAC), Mossbauer spectroscopy, among others, are widely use for the study of the properties of solids through the determination of the electric-field-gradient (EFG) tensor at the position of a probe nucleus. All these nuclear experimental techniques do not determine directly the EFG but rather one or more characteristic nuclear quadrupole resonance frequencies νQ, which are proportional to the EFG and to the nuclear quadrupole moment Q. Provided an exact value of Q for the involved nuclear state involved is known, experimental EFG information can be deduced. However, in spite of the wide use of the experimental techniques, for many important probe nuclei the exact Q value is not known with sufficient accuracy and/or precision. This is a serious problem because part of the information that νQ can provide about the system under study can be extracted only by confrontation with ab initio calculated values of the EFG. For this reason, the knowledge of reliable Q values is of great importance in atomic, molecular, and condensed-matter physics, besides the direct interest in nuclear physics, where the determination of Q values can be used to check nuclear models. Ideally, theories of the nuclear state should provide values of the nuclear quadrupole moments but often the uncertainties involved are larger than what can be accepted for the interpretation of nuclear spectroscopy experiments. Another approach involves the calculation of EFG's by ab initio electronic structure methods and comparison with experimental values of νQ frequencies. Following this approach we present a determination of the nuclear-quadrupole moment of the I=5/2+ 245 keV excited state of 111Cd. This isotope and this particular state is the most frequently used tracer in TDPAC experiments and has been largely applied to study semiconductor physics, and a large amount of experimental work has been focused on the EFG characterization at 111Cd impurity sites in metals, semiconducting, and insulating compounds. Although the importance of this isotope, the Q value of the sensitive state is known with limited precision (Q=0.83(13) b, i.e with a relative error of 17%). In this work we present ab initio calculations performed with the Full-Potential Augmented Plane Waves plus Local orbitals (APW+lo) method, considering different approximations for the exchange and correlation potential. Aiming at a very reliable determination of Q, we compared our 0 K calculations only with experimental results at very low temperatures (in the order of 4 K). Metallic and semiconducting materials were treated separately. The new value of Q that is obtained in this way will be presented and discussed.

Are you a student, a delegate from developing countries or a participant with physical needs and would like to apply for a sponsored accomodation. Please answer with yes or no.

yes

Please specify whether you would prefer an oral or poster contribution.

Poster Contribution

Primary authors: Prof. ERRICO, Leonardo Antonio (Universidad Nacional de La Plata); Prof. RENTERÍA,

Mario (Universidad Nacional de La Plata); Dr COTTENIER, Stefaan (Ghent University)

Presenters: Prof. ERRICO, Leonardo Antonio (Universidad Nacional de La Plata); Prof. RENTERÍA, Mario (Universidad Nacional de La Plata); Dr COTTENIER, Stefaan (Ghent University)

Track Classification: Nuclear Moments, Nuclear Polarization, Nuclear Models, Fundamental Interactions