

# The 245 keV level of $^{111}\text{Cd}$ : nuclear quadrupole moment and its error bar

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It hardly needs justification that the 245 keV level of  $^{111}\text{Cd}$  is an important one for hyperfine interaction studies, given the prominent role of  $^{111}\text{Cd}$  as a TDPAC probe nucleus. This makes the (re)assessment of the nuclear quadrupole moment of this level a recurrent topic at the recent editions of the HFI/NQI conferences. Nobody really challenges the experimental value of 0.83(13) b obtained by Herzog et al. back in 1980[1]. Since that time, the scene has changed and a comparison between Density Functional Theory based electric-field gradients and experimental quadrupole interaction frequencies has become the method of choice for the determination of quadrupole moments of isotopes that are relevant for hyperfine interaction methods (e.g. [2, 3]). This culminated in the value of 0.765(15) b for  $^{111}\text{Cd}$ , presented by Haas and Correia [4] at the 2012 HFI/NQI conference.

A new trend in applied Density Functional Theory, is assessing in a quantitative way the error bar on predicted values (e.g. [5, 6]). In the present contribution we do not only try to achieve a numerically completely converged value for the  $^{111}\text{Cd}$  quadrupole moment, we also aim at determining the error bar on this value. This is done by calculating the electric-field gradient at a Cd nucleus in 7 elemental solids (In, Sn, Hg, Sb, Cd, Zn, Ga) with extreme settings for numerical accuracy. For these solids, accurate experimental quadrupole interaction frequencies and lattice parameters are known at low temperature. Analyzing these two data sets with a proper statistical formalism, leads to (1) a ‘new’ prediction for the  $^{111}\text{Cd}$  quadrupole moment (which is in good agreement with previous values), and – more importantly – (2) a statistically justified error bar on this quadrupole moment.

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- [1] P. Herzog, K. Freitag, M. Reuschenbach, H. Walitzki, Z. Phys. A 294 (1980) 13  
[2] P. Dufek, P. Blaha, K. Schwarz, Physical Review Letters 75 (1995) 3545  
[3] L. Errico, G. Darriba, M. Rentería, Z. Tang, H. Emmerich, S. Cottenier, Physical Review B 77 (2008) 195118 (2008)  
[4] H. Haas and J.G. Correia, Hyperfine Interactions 198 (2010) 133  
[5] K. Lejaeghere, V. Van Speybroeck, G. Van Oost, S. Cottenier, Critical Reviews in Solid State and Materials Sciences 39 (2014) 124 (open access, <http://dx.doi.org/10.1080/10408436.2013.772503>)  
[6] K. Lejaeghere, J. Jaeken, V. Van Speybroeck, S. Cottenier, Physical Review B 89 (2014) 014304

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