

Half-century old Berkeley idea now finding missing links of nuclear quadrupole moments

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ABSTRACT

There are basically two ways to determine precision values for nuclear quadrupole moments (Q): measurements for stable or reasonably long-lived (mostly ground) states by atomic and molecular spectroscopy and measurements for much shorter-lived excited states using nuclear condensed-matter techniques like Mössbauer or perturbed-angular distribution and correlation (PAC) spectroscopy. In all cases, the direct experimental result is the product of the electric-field gradient (EFG) at the nuclear site with Q. The EFG for atomic and simple molecular systems can now mostly be calculated by theory with good accuracy, while the present status of density functional calculations of solid-state systems used for short-lived excited states limits the accuracy, generally to a 10%–20% level. Thus, the EFG of at least one matrix where data for excited states exist must be calibrated by measuring a ground state with known Q using magnetic or quadrupole resonance. This procedure is obviously not applicable to elements having no stable isotope with $I > 1/2$. For Cd, the problem has now been overcome using a concept proposed in Berkeley half a century ago, measuring isolated free Cd (and Hg) molecules with PAC. A similar project for Pb ongoing at ISOLDE/CERN is sketched, as well as a related one for Sn.

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I. HISTORICAL BACKGROUND

Around 1970, the use of nuclear properties to study matter was becoming an important area of research worldwide. For stable nuclei in their ground state, the techniques of nuclear magnetic resonance (NMR) and nuclear quadrupole resonance (NQR) had been already used extensively in solid-state investigations and high-resolution microwave molecular spectroscopy was developed for free molecules. The technique of Mössbauer spectroscopy (ME) as a tool to study condensed matter using radioactive isotopes was starting to be applied in various labs, in particular also by the group of Professor David Shirley at Lawrence Berkeley Laboratory.¹ This highly active group had also performed pioneering experiments on hyperfine fields in ferromagnets using the perturbed-angular correlation (PAC)² and low temperature nuclear orientation³ techniques. The results obtained first lead to an understanding of the magnetic hyperfine fields acting on nuclei in magnetic solids.⁴ Specifically noteworthy were the first successful combinations of these techniques with NMR detection,^{5,6} as well as the first perturbed-angular

distribution (PAD) experiment⁷ supplemented in the same manner. All these efforts were concentrating on the interaction of magnetic nuclear moments (μ) with magnetic fields (B) by measuring the Larmor frequency,

$$\nu_L = B\mu/(h).$$

Of interest for the materials studied are the internal fields acting on the nuclei. These can directly be obtained from the measured ν_L since experiments with fields created by external magnets are also generally possible for normalization.

The world-wide first efficient multidetector spectrometer for PAC constructed in this laboratory was originally designed for the novel concept to study the motion of biomolecules in liquids.^{8,9} It also opened the possibility to study the nuclear quadrupole interaction (NQI) in condensed matter on a large scale. The multitude of isotopes suitable for this technique not only allowed the investigation of materials, such as metals, semiconductors, ionic and

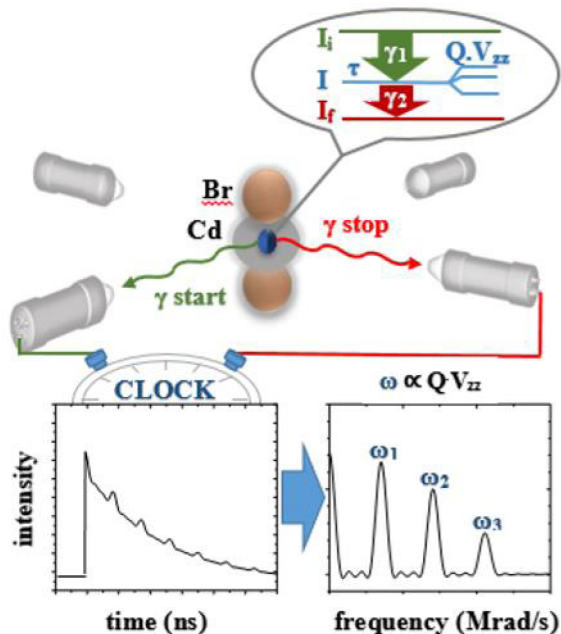


FIG. 1. Schematic explanation of PAC measurement. The Cd nucleus with quadrupole moment Q interacts with the electric-field gradient of the electrostatic potential at the nucleus $V_{zz} = \partial^2\Phi(\vec{r})/(\partial x/\partial y)$ (EFG) created by Cd electron distribution modified by bonding to the neighboring atoms (here Br). This is observed by the modulation of time distribution of the two γ rays emitted in the decay of ^{111m}Cd . The energy splitting of the nuclear intermediate state is directly seen as transition frequencies (ω) in the Fourier transform. Reproduced with permission from Haas *et al.*, Phys. Rev. Lett. **126**, 103001 (2021). Copyright 2021, American Physical Society.

molecular solids, but also liquids and high-density gases.¹⁰ Figure 1 sketches the principles of PAC measurement.

The picture of our present work-horse spectrometer (Fig. 2) could as well have been taken 50 years ago, since only the detector crystals and the computerized electronics¹¹ have changed.

The idea to apply this technique to isolated molecules as well failed at the time, however, due to technical problems,¹² as did later

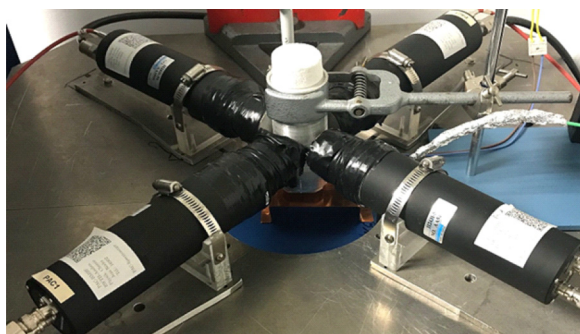


FIG. 2. Table-top setup of a typical PAC experiment.

attempts at other laboratories.¹³ The early PAC results for NQI correct such in metals at Berkeley also stimulated the introduction of the accelerator-based PAD method in this field.¹⁴

The direct experimental information from all such experiments is the nuclear quadrupole interaction constant,

$$v_Q = V_{zz} Q e/h,$$

of the nuclear quadrupole moment (Q) with the electric-field gradient (EFG), the second derivative tensor of the electronic charge density at the nucleus (V_{zz}) acting at the nucleus. Since there is no possibility to create an EFG of sufficient strength for observable interaction in the laboratory, one is forced to rely on calculating the electronic charge distribution by theoretical methods. 50 years ago such calculations were not even approximately correct. One thus had to resort to models and approximations. The uncertainty for the nuclear quadrupole moments extracted, opposite to the case of magnetic moments, therefore, was quite high. Figure 3 illustrates the situation. This severely limited the interpretation of extracted EFG, one of the few experimentally available direct measures of charge distribution in the matter, as it essentially contains information on the asymmetry in the local p- (or d-) orbitals, a property intimately related to chemical bonding.

II. ACCURACY OF EFG CALCULATIONS

Precise nuclear quadrupole moments are essential not only for any quantitative analysis of NQI measurements in solids, molecules, or atoms, but they can also contribute much to a detailed understanding of nuclei. Obviously, at least for one reference system for each element, a highly precise calculation of the EFG is an essential requisite.

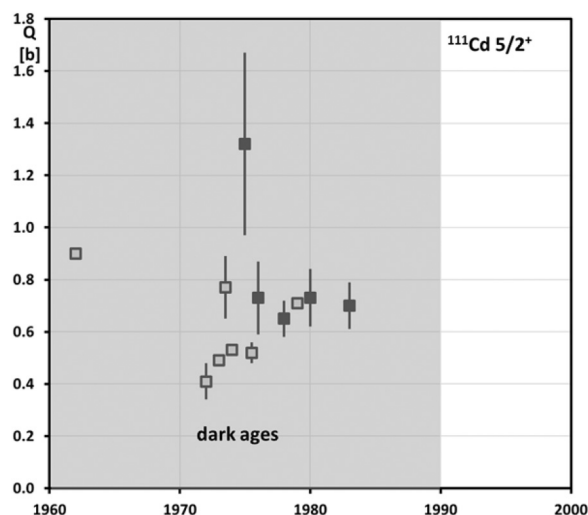


FIG. 3. Ancient history of Q for $^{111}\text{Cd } 5/2^+$. “Measurements” (black squares) and estimates (open squares).

For atomic systems, the quantum mechanical methods to calculate the EFG have by now become generally quite successful in the interpretation of data, at present mostly coming from collinear laser spectroscopy. Also, more recently, molecular data—mostly from microwave spectroscopy—have been analyzed by quantum chemistry methods that have become very precise. The present reference data¹⁵ for Q have, therefore, often reached a precision on the 1% level.

With the advent of the density functional technique (DFT), also suitable for metals,¹⁶ a possibility to routinely calculate EFGs in solids became available. For several test cases, the early results had been quite promising.^{17,18} Such calculations with a full-potential linearized augmented plane waves code WIEN2k,¹⁹ mostly using the generalized gradient approximation,²⁰ are now often performed also to calculate the EFG in solids with the aim to get an accurate Q. An example is a case of the $5/2^+$ state in ^{111}Cd , of particular importance for the interpretation of PAC measurements in condensed matter.^{21,22} It has been known for some time, however, that the standard DFT procedures severely fail to reproduce the known EFG in some cases such as Cu_2O ,²³ a semiconductor, As and Sb,²⁴ semimetals, and the asymmetry parameter η for the solid halogens,²⁵ insulators. Similarly, values found for Q from DFT calculations for halogen²⁶ or Sb²⁷ solids were systematically larger than the currently accepted ones.¹⁵ It had also become apparent that such techniques, even for simple metals, can underestimate the actual EFG by some 10%–20%.²⁸ Even more severe, the effects of intermolecular interaction may be overestimated by a factor of 2.²⁵ There is a possibility that more accurate values can be obtained with hybrid DFT calculations,²⁸ as the PBE0 method,²⁹ where a fraction of Hartree–Fock (HF) exchange is mixed to the DFT one. Such an approach, however, suffers from the inclusion of a material-dependent mixing parameter and typically requires 1000 times longer computing times.

III. MISSING-LINK PROBLEM

Considering the present status of theoretical precision for EFG calculations, the analysis of experimental measurements with an aim to obtain accurate values for Q from the atomic or molecular data may be considered satisfactory in most cases, though more careful calculations might still be required in some problem cases.

There are, however, almost as many attempts to measure the nuclear moments for short-lived excited states in the 1 ns to 1 ms lifetime range as for the long-lived cases, as shown in Fig. 4. For these, on the other hand, a different approach must be taken.

It is obvious that in cases where—for at least one of the materials—a precise measurement for an excited state is available, the EFG for the corresponding element can be normalized by measuring it for a ground state with techniques such as NQR, NMR, or ME. The problem is thus solved. This technique to link the measurements of short-lived states to those of long-lived ones evidently only works for the “easy” cases, where a stable isotope with spin greater than 1/2 is available. As demonstrated in Fig. 5, this has been accomplished with reasonable accuracy in most of these cases.

That leaves the “missing link” cases, where no suitable stable isotope is available. We have started to attack some of these in projects at the ISOLDE isotope separator³⁰ using the idea discussed

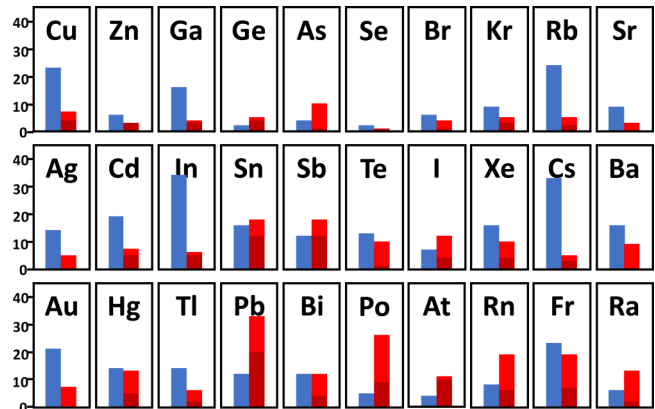


FIG. 4. Extent of the problem linking existing quadrupole moment data for the number of long-lived states (blue, left column) to short-life state measurements (red, right column).

some 50 years ago in Berkeley,¹⁰ to measure the isolated molecules by PAC.

IV. Cd, Hg, AND Zn ISOTOPES

During the last decade, a more advanced extension of the standard DF methods, the admixture of some HF exchange to the DF,³¹ has been very successfully applied in chemical research. Such hybrid calculations for solids have also recently solved a long-standing problem of standard DF calculations, the failure to reproduce electronic gaps in semiconductors and insulators.^{32,33} It has been noted that this procedure significantly changes the computed EFG as well.³⁴

We had, therefore, first applied the hybrid DFT in a redetermination of Q for Cd and Zn. By combining the results with new calculations for molecules [$\text{Cd}(\text{CH}_3)_2$, ZnS] and atoms ($^3\text{P}_1$ state of Zn), we have arrived at a consistent picture for Q in both cases, resulting in a substantial shift (more than 15%)³⁵ from the previously accepted values. This achievement has solved a problem that

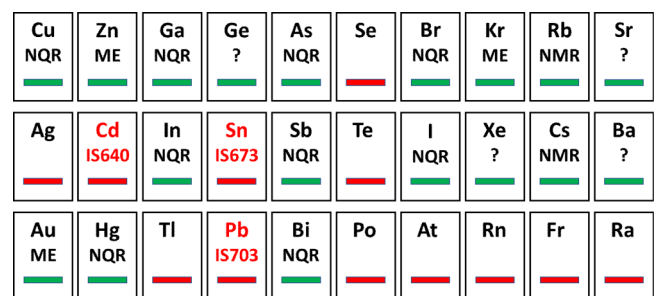


FIG. 5. Easy (underlined) and problem (red) cases for linking solid state to atomic or molecular data. The ISOLDE/CERN projects (Cd, Sn, Pb) discussed here are shown.

has been around for some 50 years to a large degree, demonstrated by the history for the Q of ^{111}Cd summed in Fig. 3. As final values, we reached,

$$Q(^{111}\text{Cd } 5/2^+) = 0.641(25) \text{ b and } Q(^{67}\text{Zn gs}) = 0.125(5) \text{ b,}$$

the major uncertainty involved for Cd is the estimation of the effect of intermolecular interactions in solid Cd-dimethyl.

This then raised the old idea to measure free molecules, where the intermolecular interaction does not exist, to a project IS640 at ISOLDE/CERN. The basic idea of this concept was the fact that for rotating free linear molecules, the rotational angular momentum J is always perpendicular to the molecular axis. Thus, the tensor component of the (traceless) EFG tensor is minus 1/2 the molecular one along the bond direction. Therefore, for large J , one should expect to see a PAC perturbation with half the frequency (twice the period) of a fixed molecule. The technical problem then boils down to the production of samples where the free flight time of the radioactive molecules is long compared to the measurement time.

The idea was first tested with sources of $^{199\text{m}}\text{Hg}$, where the half-life of the $5/2^-$ intermediate state is only 1.8 ns. The obtained spectra³⁶ shown in Fig. 6 clearly demonstrate the predicted behavior, as well as the well-known effect of additional gas collisions.

In quantitative analysis, the obtained values for EFG in the HgCl_2 and HgI_2 molecules are in complete agreement with the results of CCSD-T calculations available from an earlier work,³⁷ in

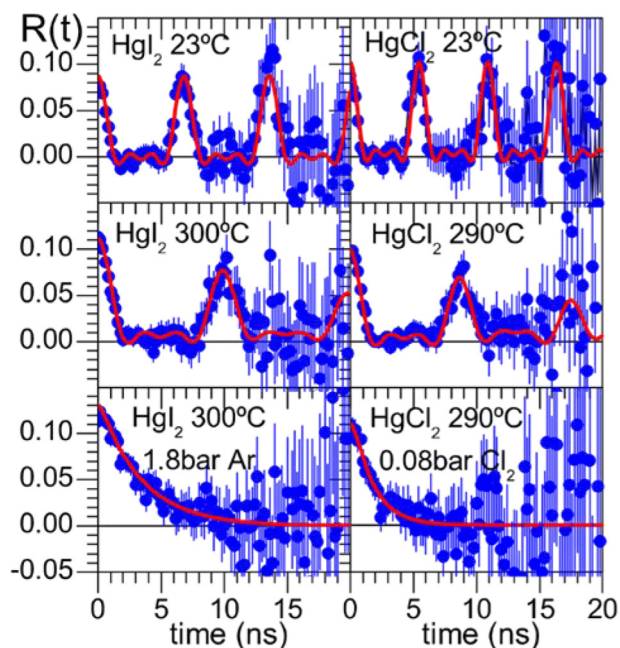


FIG. 6. Observed PAC patterns for Hg halides at room temperature (top), in the gas phase (middle), and with additional other gas (bottom) (blue points: data, red lines: theory). Reproduced with permission from Haas *et al.*, Phys. Rev. Lett. **126**, 103001 (2021). Copyright 2021, American Physical Society.

this manner also confirming the well-known Q for this state^{38,39} and the basic concept of the project. Of additional interest is that, in these cases, the corresponding solids also crystallize as an assembly of molecules. The effects of intermolecular interaction on the EFG are, however, quite strong for these materials, in disagreement with the expectation from earlier DFT calculations.^{39,40} A more comprehensive theoretical analysis of these unique experimental results is still to be performed.

The corresponding measurements using $^{111}\text{Cd } 5/2^+$ in three Cd halides were technically much more demanding due to the considerably longer state half-life of 80 ns, the higher measuring temperatures needed, and the lower thermal molecular stability.

The high quality of the obtained spectra³⁶ shown in Fig. 7 allows to clearly see the three (practically) equidistant transition frequencies in the Fourier transform, as expected for the nuclear spin $5/2$. In the detailed theoretical analysis, small contributions of vibrational excitation, centrifugal stretching, and the quantum nature of the coupling of the nuclear spin I to the rotational J had to be included. The value of Q obtained from the data for the three dihalides obtained, when compared with new CCSD-T calculations, is practically the same. Figure 8 shows the progress in precision achieved in getting to

$$Q(^{111}\text{Cd } 5/2^+) = 0.664(8) \text{ b.}$$

V. Pb, In, AND Ge ISOTOPES

Using the method applied for ^{111}Cd to the other state well suited for PAC, the 4^+ level in ^{204}Pb should be quite straightforward in principle, and a project IS703 is proposed to do exactly that by measuring PbO and other Pb chalcogenides. Due to the even longer state half-life of 280 ns, the higher spin, and still higher measuring temperatures required, the technical problems will be more severe, however. Considering the importance of accurate numbers of Q , in the interpretation of the abundant experimental frequency data available for the excited states in closed-proton shell Pb isotopes (cf. Fig. 4), it will be worthwhile to attempt.

For the series of Sn isotopes, where a similar situation exists, measurements in the gas phase using the excited $3/2^+$ state in ^{119}Sn appear quite out of range at the moment. Fortunately, in the abundant literature on this state, widely used in Mössbauer spectroscopy, there are a few NQI data for matrix-isolated molecules. We have made a preliminary analysis of such information for SnO that shows the Q now recommended¹⁵ as grossly wrong. This finding will, however, have to be augmented by more precise frequency ratio measurements to other excited states (project IS673) for a consistent picture.

For the Ge isotopes, in principle, it should be “easy” to link the existing measurements for several excited states to the known Q of the ^{73}Ge ground state. Unfortunately, the experiments one could envision using ME or NMR are quite challenging. One, thus, will presumably be forced to rely on an improved solid-state theory of the EFG for Ge as an impurity in solids like Zn, Cd, or Sn to improve the existing attempt.⁴¹ Equivalent calculations of the EFG at neighboring impurity elements with now precisely known Q could serve as a reliability check of such an approach.

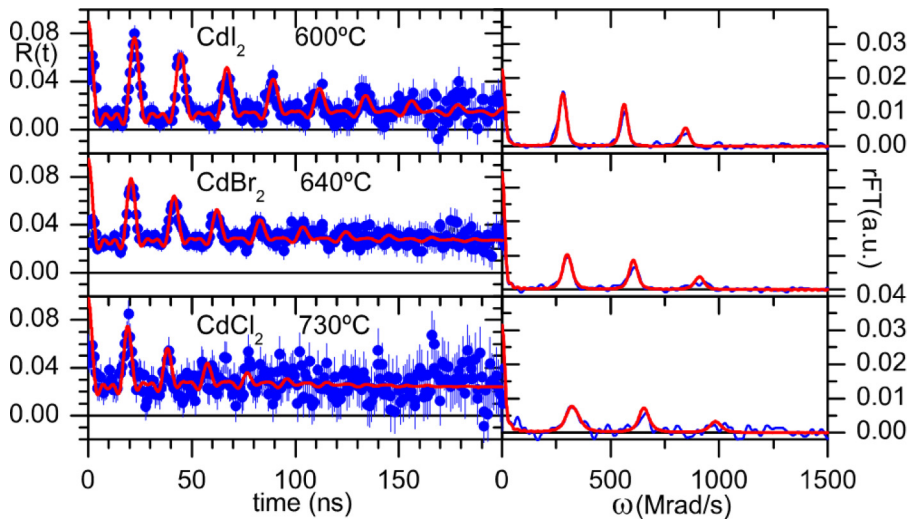


FIG. 7. Observed PAC patterns for Cd halides in the gas phase. The Fourier transforms (right) clearly show the three frequencies typical for nuclear spin 5/2. Reproduced with permission from Haas *et al.*, Phys. Rev. Lett. **126**, 103001 (2021). Copyright 2021, American Physical Society.

VI. IMPLICATIONS FOR NUCLEAR THEORY

The nuclear moments for high-spin states often show a remarkable simplicity as a function of neutron number. A particular example are the quadrupole moment values of the $11/2^-$ states in Cd isotopes. They have long been known to change very systematically, and the linear trend for heavier isotopes had actually been applied in the early estimations of Q for the ^{111}Cd $5/2^+$ state from the results of PAD experiments.^{42,43} This linear trend has recently been confirmed by high precision collinear laser spectroscopy⁴⁴ and then explained within the nuclear covariant density functional theory (CDFT).⁴⁵ Since the PAD experiments relate the quadrupole moments of the short-lived $11/2^-$ states in $^{107,109}\text{Cd}$ accurately to

that of ^{111}Cd $5/2^+$, determined with high precision, we can now further extend the observed trend. In Fig. 9, a saturation of the quadrupole moments is clearly demonstrated for $^{107,109}\text{Cd}$.

This saturation is fully consistent with the prediction from new nuclear calculations³⁵ with the same CDFT procedure used earlier for the heavier isotopes. The obvious agreement with the experimental results there is very satisfactory. However, the

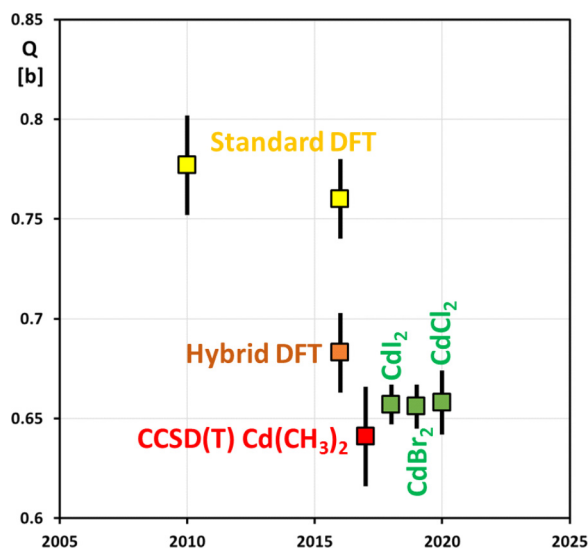


FIG. 8. Final results for Q of ^{111}Cd $5/2^+$.

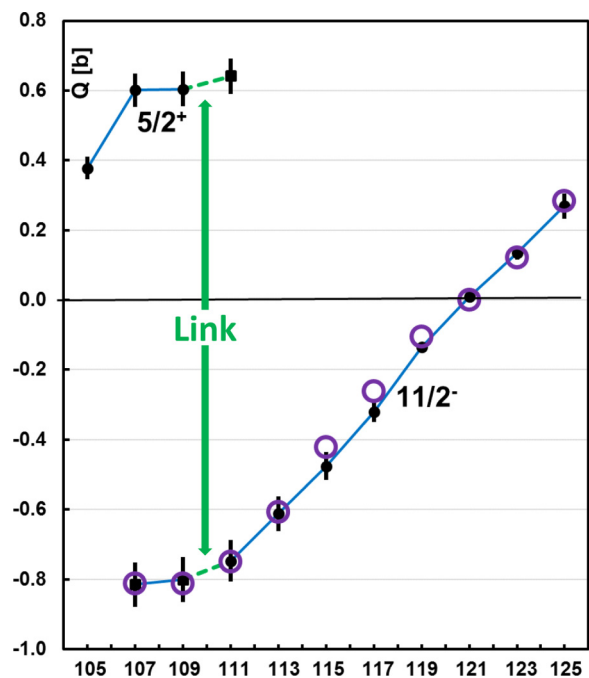


FIG. 9. Systematics for Q of $11/2^-$ and $5/2^+$ states in Cd isotopes, demonstrating the importance of linking atomic (black dots) to solid-state (black squares) data. The circles are from the theory.

emerging trend for the $5/2^+$ states—hopefully soon augmented by new laser spectroscopy ($^{99,101,103,105}\text{Cd}$) and PAC (^{113}Cd) data—will require a more microscopic nuclear theory approach.

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AUTHOR DECLARATIONS

Conflict of Interest

The author has no conflicts to disclose.

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

REFERENCES

- ¹D. Salomon, G. Kaindl, and D. A. Shirley, *Phys. Lett. A* **36**, 457 (1971).
- ²E. Matthias, S. S. Rosenblum, and D. A. Shirley, *Phys. Rev. Lett.* **14**, 46 (1965).
- ³G. A. Westenbarger and D. A. Shirley, *Phys. Rev.* **138**, A161 (1965).
- ⁴R. B. Frankel, J. Huntzicker, E. Matthias, S. S. Rosenblum, D. A. Shirley, and N. J. Stone, *Phys. Lett.* **15**, 163 (1965).
- ⁵E. Matthias D. A. Shirley, M. P. Klein, and N. Edelstein, *Phys. Rev. Lett.* **16**, 974 (1966).
- ⁶J. A. Barclay *et al.*, *J. Appl. Phys.* **39**, 1243 (1968).
- ⁷D. Quitmann, J. M. Jaklevic, and D. A. Shirley, *Phys. Lett. B* **30**, 329 (1969).
- ⁸T. K. Leipter, J. D. Baldeschwieler, and D. A. Shirley, *Nature* **220**, 907 (1968).
- ⁹D. A. Shirley, *J. Chem. Phys.* **53**, 465 (1970).
- ¹⁰H. Haas and D. A. Shirley, *J. Chem. Phys.* **58**, 3339 (1973).
- ¹¹C. Herden, J. Röder, J. A. Gardner, and K. D. Becker, *Nucl. Instrum. Methods Phys. Res., Sect. A* **594**, 155 (2008).
- ¹²H. H. Rinneberg and D. A. Shirley, private communication (December 12, 1972).
- ¹³F. Reuschenbach, Diplomarbeit (University of Bonn, 1977).
- ¹⁴J. Bleck, R. Butt, H. Haas, W. Ribbe, and W. Zeitz, *Phys. Rev. Lett.* **29**, 1371 (1972).
- ¹⁵P. Pyykkö, *Mol. Phys.* **116**, 1328 (2019).
- ¹⁶P. Blaha, K. Schwarz, and P. H. Dederichs, *Phys. Rev. B* **37**, 2792 (1988).
- ¹⁷P. Blaha *et al.*, *Hyperfine Interact.* **97**, 1 (1996).
- ¹⁸H. Haas and H. M. Petrilli, *Phys. Rev. B* **61**, 13588 (2000).
- ¹⁹P. Blaha *et al.*, *WIEN2k: An Augmented Plane Wave plus Local Orbitals Program for Calculating Crystal Properties* (Vienna University of Technology, Austria, 2018).
- ²⁰J. P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* **77**, 3865 (1996).
- ²¹H. Haas and J. G. Correia, *Hyperfine Interact.* **198**, 133 (2010).
- ²²L. Errico, K. Lejaerghere, J. Runco, S. N. Mishra, M. Rentería, and S. Cottenier, *J. Phys. Chem. C* **120**, 23111 (2016).
- ²³R. Laskowski, P. Blaha, and K. Schwarz, *Phys. Rev. B* **67**, 075102 (2003).
- ²⁴G. L. Hill, J. M. Kearnland, M. J. R. Hoch, and H. Haas, *Phys. Rev. B* **58**, 13614 (1998).
- ²⁵H. Haas, *Hyperfine Interact.* **197**, 17 (2010).
- ²⁶R. E. Alonso, A. Svane, C. O. Rodriguez, and N. E. Christensen, *Phys. Rev. B* **69**, 125101 (2004).
- ²⁷A. Svane, *Phys. Rev. B* **68**, 064422 (2003).
- ²⁸H. Haas, M. B. Barbosa, and J. G. Correia, *Hyperfine Interact.* **237**, 115 (2016).
- ²⁹J. P. Perdew, M. Ernzerhof, and K. Burke, *J. Chem. Phys.* **105**, 9982 (1996).
- ³⁰R. Catherall *et al.*, *J. Phys. G* **44**, 094002 (2017).
- ³¹J. Heyd, G. E. Scuseria, and M. Ernzerhof, *J. Chem. Phys.* **118**, 8207 (2003).
- ³²J. Heyd, J. E. Peralta, G. E. Scuseria, and R. L. Martin, *J. Chem. Phys.* **123**, 174101 (2005).
- ³³M. A. L. Marques, J. Vidal, M. J. T. Oliveira, L. Reining, and S. Botti, *Phys. Rev. B* **83**, 035119 (2011).
- ³⁴F. Tran and P. Blaha, *Phys. Rev. B* **83**, 235118 (2011).
- ³⁵H. Haas, S. P. A. Sauer, L. Hemmingsen, V. Kellö, and P. W. Zhao, *EPL* **117**, 62001 (2019).
- ³⁶H. Haas *et al.*, *Phys. Rev. Lett.* **126**, 103001 (2021).
- ³⁷V. Arcisauskaitė, S. Knecht, S. P. A. Sauer, and L. Hemmingsen, *Phys. Chem. Chem. Phys.* **14**, 2651 (2012).
- ³⁸J. Bieron, P. Pyykkö, and P. Jönsson, *Phys. Rev. A* **71**, 012502 (2005).
- ³⁹W. Tröger, T. Butz, P. Blaha, and K. Schwarz, *Hyperfine Interact.* **80**, 1109 (1993).
- ⁴⁰T. Soldner, W. Tröger, T. Butz, P. Blaha, and K. Schwarz, *Z. Naturforsch., A: Phys. Sci.* **53**, 411 (1998).
- ⁴¹H. Haas and J. G. Correia, *Hyperfine Interact.* **197**, 11 (2010).
- ⁴²O. Echt, H. Haas, E. Ivanov, E. Recknagel, E. Schlodder, and B. Spellmeyer, *Hyperfine Interact.* **2**, 230 (1976).
- ⁴³G. D. Sprouse, O. Häusser, H. R. Andrews, T. Faestermann, J. R. Beene, and T. K. Alexander, *Hyperfine Interact.* **4**, 229 (1978).
- ⁴⁴D. T. Yordanov, *Phys. Rev. Lett.* **110**, 192501 (2013).
- ⁴⁵P. W. Zhao, S. Q. Zhang, and J. Meng, *Phys. Rev. C* **89**, 011301 (2014).