

# PAC studies of isolated small Cd and Hg molecules: The nuclear quadrupole moments

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\* Spokespersons

## What we would like to do:

- Measure the quadrupole interaction in some free Cd (and Hg) molecules in the gas state by PAC
- Basic idea: In a linear molecule the EFG ( $V_{zz}^{\text{mol}}$ ) is along the molecular axis
- The rotation axis J is always perpendicular to the molecular axis
- The EFG along J is then, independent of J:

$$V_{zz}^{\text{rot}} = -1/2 V_{zz}^{\text{mol}}$$

- For large J the quantization should be fully along J, leading to a splitting frequency independent of J !
- An old idea, but early experiments (Berkeley, Bonn) in the 1970s have failed

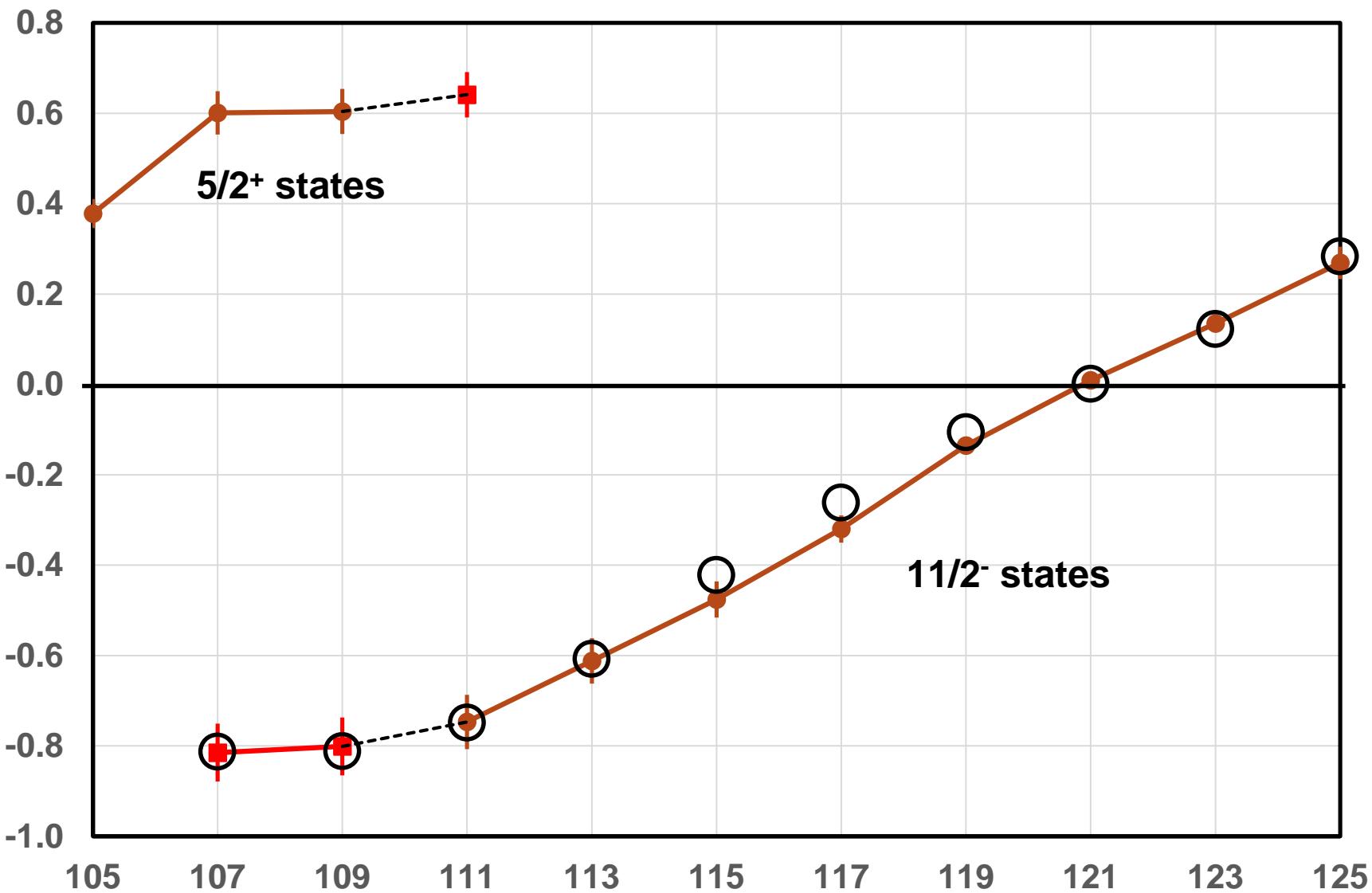
# Why now ?

**Quadrupole moments of Cd and Zn nuclei: When solid-state, molecular,  
atomic, and nuclear theory meet**

**H. Haas<sup>1,5\*</sup>, S.P.A. Sauer<sup>2</sup>, L. Hemmingsen<sup>2</sup>, V. Kellö<sup>3</sup>, and P.W. Zhao<sup>4</sup>**

- What we have done:
- Calculated the EFG in a simple molecule  $\text{Cd}(\text{CH}_3)_2$  with quantum chemistry techniques and extracted Q for  $^{111}\text{Cd}$   $5/2^+$
- Extended series of Q for  $11/2^-$  states by combining with old PAC and PAD data

# Cd Quadrupole moments



# Why now ?

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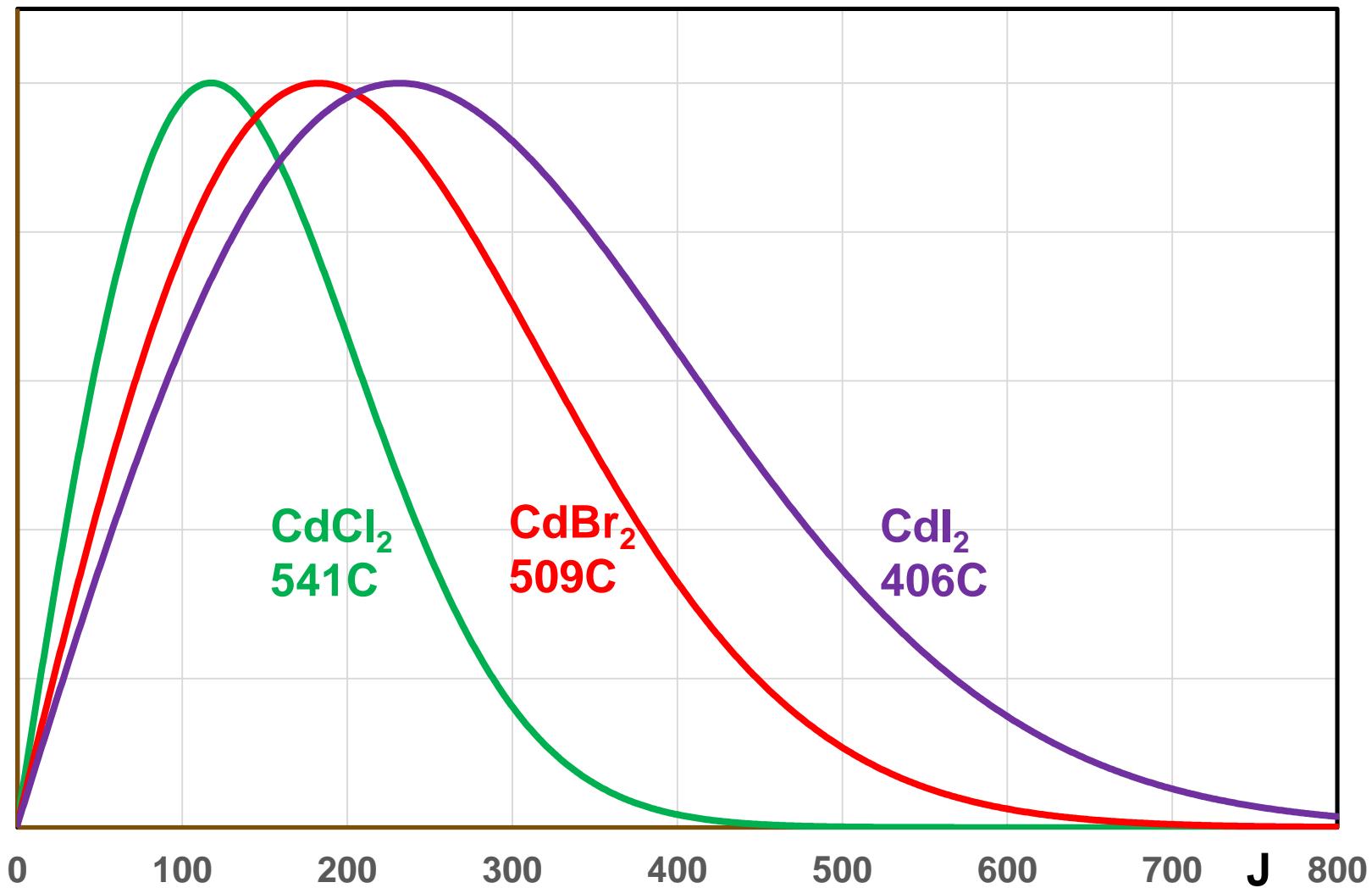
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- Theory (nuclear covariant density functional calculations) nicely confirms the observed saturation of Q at  $^{109}\text{Cd}$
- **But !** The experimental quadrupole interaction is only known for the molecular solid, requiring a (somewhat uncertain) correction for solid-state effects
- Conclusion: Measure free molecules !

# Candidate molecules

	mp	bp	R	$n_O^{mol}$	$n_O^{sol}$	$T_{exp}$	$t_{PAC}$	$t_{col}$	$p_{max}$	
	[C]	[C]	[Å]	[MHz]	[MHz]	[C]	[ns]	[ns]	[hPa]	
$CdCl_2$	564	964	2.282	406	49.2	541	130	3.10	25	
$CdBr_2$	568	863	2.394	368	24.6	509	150	3.52	25	
$CdI_2$	388	744	2.582	367	9.7	406	151	3.77	24	
$HgCl_2$	276	304	2.252	1272	1235	131	42	5.51	120	
$HgBr_2$	236	322	2.383	1154	1030	132	46	5.68	110	
$HgI_2$	259	350	2.554	1152	63	152	46	5.42	110	

# Population of J states



# Quantum mechanics

- No J:  $\hat{H} = eQV_{zz} \left\{ \frac{3I_z^2 - I(I+1)}{4I(2I-1)} \right\}$
- $R(t) = a_0 + a_1 \cos(w_0 t) + a_2 \cos(2w_0 t) + a_3 \cos(3w_0 t)$
- $w_0 = \frac{6}{4I(2I-1)} \frac{eQV_{zz}}{h}$

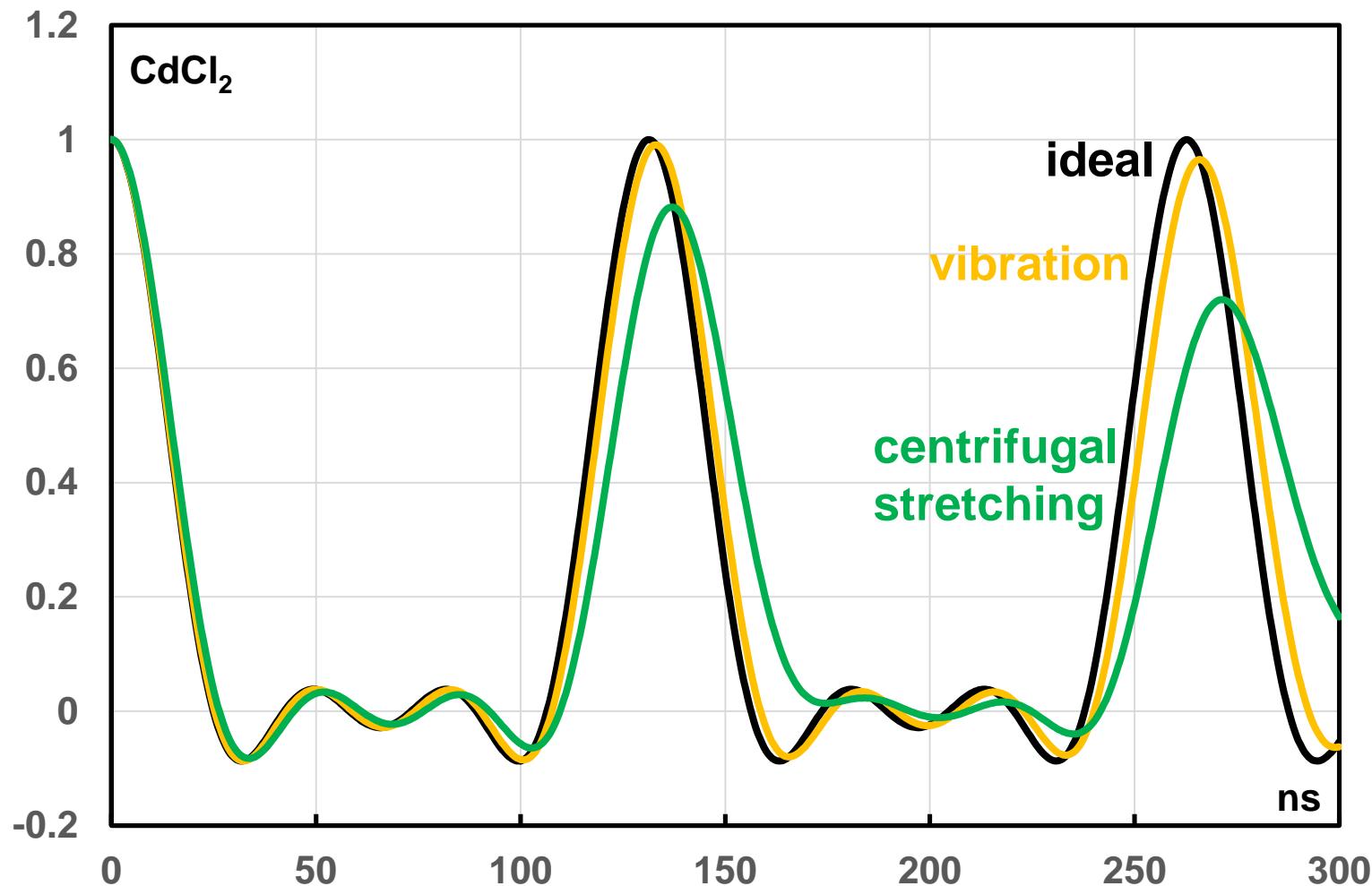
# Quantum mechanics

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- $w_0 = \frac{6}{4I(2I-1)} \frac{eQV_{zz}}{h}$
- With J:  $\hat{H} = eQV_{ZZ} \left\{ \frac{3(I_J)^2 + 1.5(I_J) - J(J+1)I(I+1)}{2J(2J-1)4I(2I-1)} \right\}$
- Casimir formula (1933)

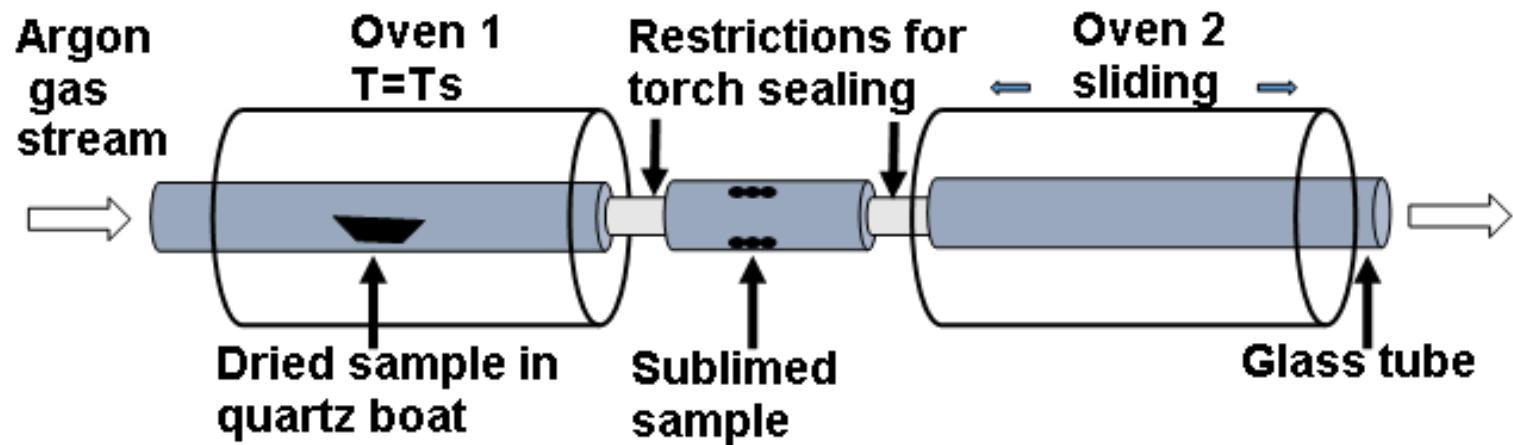
# Quantum mechanics

- No J:  $\hat{H} = eQV_{zz} \left\{ \frac{3I_z^2 - I(I+1)}{4I(2I-1)} \right\}$
- $R(t) = a_0 + a_1 \cos(\omega_0 t) + a_2 \cos(2\omega_0 t) + a_3 \cos(3\omega_0 t)$
- $\omega_0 = \frac{6}{4I(2I-1)} \frac{eQV_{zz}}{h}$
- With J:  $\hat{H} = eQV_{ZZ} \left\{ \frac{3(IJ)^2 + 1.5(IJ) - J(J+1)I(I+1)}{2J(2J-1)4I(2I-1)} \right\}$
- For large J:  $w = \frac{1}{4} w_0$

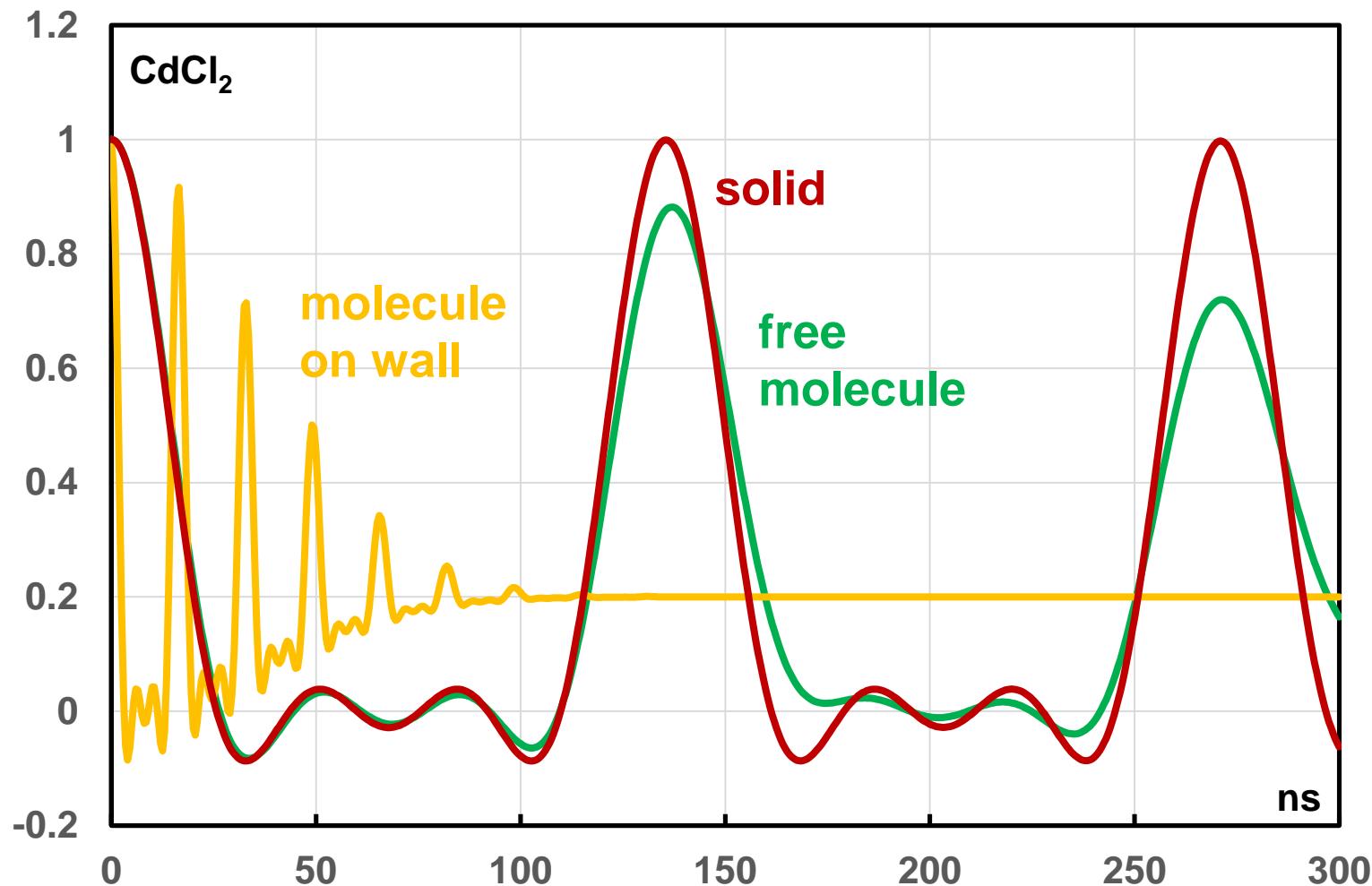
# Simulated PAC Spectrum CdCl<sub>2</sub>



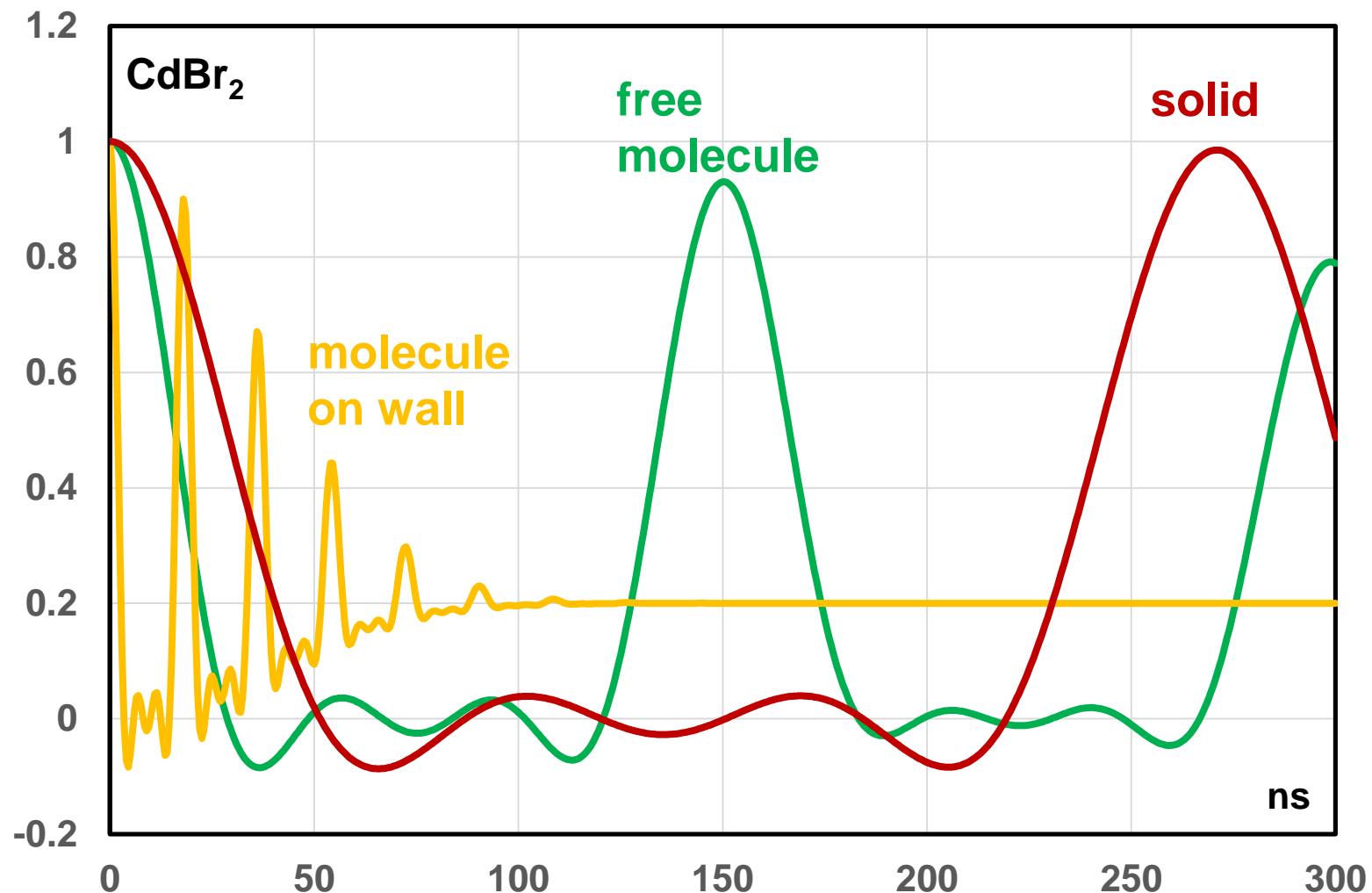
# The Technique



# Simulated PAC Spectrum CdCl<sub>2</sub>



# Simulated PAC Spectrum CdBr<sub>2</sub>



## Summary and Future (?)

- We plan the first (successful) PAC experiments on free molecules
- Goal: A precision value of Q for the  $5/2^+$  state in  $^{111}\text{Cd}$
- Test of the procedure and the quantum chemistry calculations with  $^{199}\text{Hg}$
- Possible further candidate:  $^{204}\text{PbO}$
- Other (future) technique: PAC on matrix isolated complex molecules

# Beam Time Request

Required isotope	Implanted beam	Probe element	Type of experiment	Intensity [at/ $\mu$ C]	Target / Ion source	Atoms per sample	nº of shifts
$^{111m}\text{Cd}$ (48 min)	$^{111m}\text{Cd}$	$^{111}\text{Cd}$	$\gamma$ - $\gamma$ PAC	$10^8$	Molten Sn/ VADIS	$2 \times 10^{10}$	2 x 3
$^{199m}\text{Hg}$ (43 min)	$^{199m}\text{Hg}$	$^{199}\text{Hg}$	$\gamma$ - $\gamma$ PAC	$10^9$	Molten Pb/ VADIS	$2 \times 10^{10}$	2 x 3