Nuclear Schiff moment of the fluorine isotope $^{19}\mathbf{F}$

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Nuclear Schiff moment of the fluorine isotope ^{19}F

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Nuclear Schiff moments (NSMs) are sensitive probes for physics beyond the Standard Model of particle physics, signaling violations of time-reversal and parity-inversion symmetries in atomic nuclei. In this Letter, we report the first-ever calculation of a NSM in a nuclear *ab initio* framework, employing the no-core shell model to study the fluorine isotope ^{19}F. We further perform quantum-chemistry calculations to evaluate the sensitivity of the hafnium monofluoride cation, HfF^+, to the NSM of ^{19}F. Combined with recent high-precision measurements of the molecular electric dipole moment of HfF^+ [1], our results enable the first experimental bound on the NSM of ^{19}F.

Introduction

- Rapid advancements in the control and manipulation of individual quantum states in atoms and molecules have supercharged progress in the fields of quantum information, quantum simulation, and the probing of chemical reactions at the quantum level.

- Over the years, numerous experiments have leveraged these quantum-enabled technologies to probe for electric dipole moments (EDMs) of elementary and composite particles.

- Measurements of EDMs can help constrain the nature of new physics and guide us to a better understanding of the underlying mechanisms of the universe.

One example of an EDM sensitive to fundamental symmetry violations is the molecular EDM induced by a nuclear Schiff moment (NSM) of a constituent atom, e.g., ^{19}F in HfF$^+$. The physics of the NSM has been covered comprehensively in literature, e.g., Refs. [21–26]. In brief, the NSM arises from nuclear electric moments that are only partially screened by the surrounding electron cloud due to relativistic effects and the finite size of the nucleus [27, 28]. Parity-inversion ($\mathcal{P}$) and time-reversal ($\mathcal{T}$) violation within the atomic nucleus can generate a NSM, which in turn induces a measurable EDM in atoms and molecules. While $\mathcal{P},\mathcal{T}$-violating effects predicted by the Standard Model produce EDMs well below current experimental sensitivity, many beyond-Standard-Model scenarios predict enhancements potentially within reach of ongoing or near-future measurements. As such, EDM experiments provide powerful probes of new $\mathcal{P},\mathcal{T}$-violating physics.

- EDMs of nuclei, atoms and molecules are excellent probes of new sources of CP violation.

CP violation in Standard Model:

- Phase in the CKM matrix

A. Hocker et al., Rev. Nucl. ParZ. Ligeti, Annt. Sci. 56 (2006) 501.

- Mass of neutrino → analogous leptonic CP violation

H. Nunokawa et al., Prog. Part. Nucl. Phys. 60 (2008) 338.

- $\bar{\theta}$ term in QCD

R. Jackiw, C. Rebbi, PRL 37 (1976) 172.

P, T-violating & experimental observations

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- The molecular sensitivity coefficient (W_S) which relates the observed EDM to the NSM (S), and a nuclear structure calculation that connects the NSM to the underlying P, T -violating physics.
- The energy shift, ΔE_{NSM}, of a molecular state due to the NSM of a constituent nucleus is given by,

$$\Delta E_{\mathrm{NSM}} = W_S\, S \left\langle \frac{\mathbf{I}\cdot\hat{n}}{I} \right\rangle , \tag{1}$$

State-of-the-art relativistic quantum chemistry methods, using *ab initio* approaches and extended basis sets, can determine molecular sensitivity factors with high accuracy and uncertainties at the sub-10% level [29–33].

In contrast, solving the nuclear many-body problem with comparable precision remains a major theoretical challenge, particularly when linking nuclear structure to searches for new physics. Traditionally, this connection has relied on phenomenological nuclear models that, while powerful, are typically finely tuned and model-dependent.

- The results for NSMs can vary by an order of magnitude and even disagree in sign.

J. Engel, Annual Review of Nuclear and Particle Science 75 (2025).

- Underscoring the need for more systematic and predictive nuclear theory.

$$S = a_0 g\bar{g}_0 + a_1 g\bar{g}_1 + a_2 g\bar{g}_2.$$

Table 2 The coefficients a_i in ^{211}Rn from several nuclear-structure calculations[a]

Method (reference)	a_0	a_1	a_2
Independent particles (71)	0.12	0.12	0.24
Phenomenological RPA (71)	0.0019	−0.061	0.053
Skyrme linear response (70)	0.034 ↔ 0.042	−0.0004 ↔ −0.028	0.064 ↔ 0.078

Table 3 The coefficients a_i for ^{199}Hg from several nuclear-structure calculations[a]

Method (reference)	a_0	a_1	a_2
Independent particles (49)	0.087	0.087	0.174
Pair-truncated shell model (74)	0.011	0.014	0.033
Pair-truncated shell model (75)	0.017	−0.016	0.066
Large-scale shell model (56)	0.080	0.078	0.15
Phenomenological RPA (71, 72)	0.00004	0.055	0.009
Skyrme QRPA (73)	0.002 ↔ 0.010	0.057 ↔ 0.090	0.011 ↔ 0.025
Skyrme linear response (70)	0.009 ↔ 0.041	−0.027 ↔ +0.005	0.009 ↔ 0.024

[a]Coefficients are in units of $|e|$ fm^3.

- In particular, chiral effective field theory (χEFT) provides a systematic framework that connects the symmetries of quantum chromodynamics to low-energy nuclear interactions, enabling controlled expansions of nuclear forces at the scale where protons and neutrons form atomic nuclei.

- These interactions are now routinely used in nuclear *ab initio* calculations, offering high precision and reliable uncertainty quantification. Extending ab initio methods to the calculation of NSMs thus holds promise for improving the theoretical reliability of NSM estimates.

This work

- The first nuclear ab initio calculation of a NSM, focusing on the fluorine isotope ^{19}F by using no-core shell model (NCSM).
- ^{19}F exhibits a low-lying opposite-parity excited state ($I^{\pi} = 1/2^{-}$) just ≈ 110 keV above its $1/2^{+}$ ground state.
- Show the recent high-precision measurement of the molecular EDM in HfF^{+} , while primarily constraining the electron EDM, can also be interpreted as a stringent limit on the NSM of ^{19}F. To support this, we also perform quantum-chemistry calculations of the molecular sensitivity factor for HfF^{+} and other fluorine-containing molecules.

Nuclear Schiff moment of ^{19}F

- Two sets of parity conserving (PC) χEFT nucleon-nucleon (NN) and three nucleon (3N) interactions: $\mathrm{NN}-\mathrm{N^3LO}+3\mathrm{N}_{lnl}$ and $\mathrm{NN}-\mathrm{N^4LO}+3\mathrm{N}^*_{lnl}$

$$\mathbf{S}=\frac{e}{10}\sum_{p=1}^{Z}\left(r_p^2-\frac{5}{3}\langle r^2\rangle_{\mathrm{ch}}\right)\mathbf{r}_p\ , \qquad (2)$$

- The Schiff moments are evaluated by computing the matrix elements:

$$S=\langle A,\mathrm{g.s.},I^\pi,I_z{=}I|\,S_z\,|A,\mathrm{g.s.},I^\pi,I_z{=}I\rangle+\mathrm{h.c.}, \qquad (3)$$

$$(E^{I^\pi}_{\mathrm{g.s.}}-H)|A,\mathrm{g.s.},I\rangle=V^{\mathrm{PTV}}_{\mathrm{NN}}|A,\mathrm{g.s.},I^\pi\rangle\ , \qquad (4)$$

$$S\simeq\sum_{i\neq 0}\frac{\langle\Phi_0|\hat{S}_z|\Phi_i\rangle\langle\Phi_i|\hat{V}_{PT}|\Phi_0\rangle}{E_0-E_1}+c.c.$$

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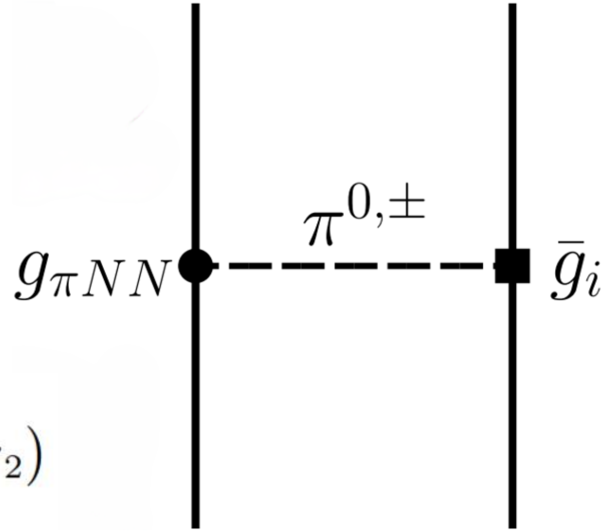
$$\mathcal{L}_{\pi N}^{(PT-even)} = -\frac{g_\pi NN}{2m_N}\bar{N}(\sigma\cdot\nabla)\vec{\tau}\cdot\vec{\pi}N$$

$$\mathcal{L}_{\pi N}^{(PT-odd)} = \bar{N}\left[\bar{g}_0\vec{\tau}\cdot\vec{\pi} + \bar{g}_1\pi^0 + \bar{g}_2(3\tau_3\pi^0 - \vec{\tau}\cdot\vec{\pi})\right]N$$



$$V_{PT} = \frac{g_{\pi NN}}{8\pi m_N}\left\{\left[\bar{g}_0\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 - \frac{\bar{g}_1}{2}(\tau_{1z}+\tau_{2z}) + \bar{g}_2(3\tau_{1z}\tau_{2z} - \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2\right](\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2)\right.$$
$$\left. - \frac{\bar{g}_1}{2}(\tau_{1z}-\tau_{2z})(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\right\}\cdot(\nabla_1-\nabla_2)\frac{\exp\left(-m_\pi|\boldsymbol{r}_1-\boldsymbol{r}_2|\right)}{m_\pi|\boldsymbol{r}_1-\boldsymbol{r}_2|}$$

- The NSM of ^{19}F is significantly enhanced compared to other light nuclei due to the presence of a relatively low-lying opposite-parity partner of its ground state and a large Schiff operator matrix element between the two states.

$$S(^{19}\mathrm{F}) = (-4.3\,g\bar{g}_0 - 3.1\,g\bar{g}_1 - 1.4\,g\bar{g}_2)\times 10^{-2}\ e\ \mathrm{fm}^3,\ (5)$$

- However, the lighter mass of ^{19}F results in smaller coefficients for the πNN coupling terms than those in heavier and octupole-deformed nuclei such as ^{225}Ra and ^{227}Ac.
- Nevertheless, the light mass of ^{19}F enables its NSM to be computed using ab initio methods that provide a more detailed and reliable description of the nuclear structure than approaches typically used for heavier nuclei.

TABLE I. Coefficients of $g\bar{g}_i$, in units of $e\,\mathrm{fm}^3$, in the expression Eq. (5) for the Schiff moment of ^{225}Ra, calculated with the SkO′ Skyrme interaction. The abbreviation "src" stands for "-short-range correlations."

	a_0	a_1	a_2
Zero range (direct only)	−5.1	10.4	−10.1
Finite range (direct only)	−1.9	6.3	−3.8
Finite range + src (direct only)	−1.7	6.0	−3.5
Finite range + src (direct+exchange)	−1.5	6.0	−4.0

J. Dobaczewski et al,. PRL 94, 232502 (2005)

	a_0	a_1	a_2	b_1	b_2
^{227}Ac	4.4(10)	−14.0(18)	8.3(31)	−0.2(2)	0.3(3)

Table 1 Sensitivity coefficients (in units of $e\,\mathrm{fm}^3$) of the laboratory Schiff moment of ^{227}Ac to the isoscalar (a_0), isovector (a_1), and isotensor (a_2) CP-odd pion-nucleon coupling constants and CP-odd heavy-meson-exchange coupling constants (b_1, b_2), calculated with nuclear density functional theory in this work.

M. Athanasakis-Kaklamanakis et al., arXiv:2507.05224 (2025).

Nuclear Schiff moment of ^{19}F

- We can then assess the contribution of the lowest opposite-parity partner, which is typically the only contribution considered in heavy systems.
- The contribution of the nuclear EDM of ^{19}F is negligible. Since the $1/2^+$ ground state is a shell-model like state with large S-wave $^{18}O + p$ amplitude while the $1/2_1^-$ state exhibits α-clustering with large S-wave $^{15}N + \alpha$ amplitude and a negligible $^{18}O + p$ amplitude.
- The matrix elements of the E1 operator and of the second term of the Schiff operator in Equation (2) ($\propto \mathbf{r}$) are very small while that of the first term of the Schiff operator ($\propto r^2\mathbf{r}$) is enhanced

$$\mathbf{S} = \frac{e}{10}\sum_{p=1}^{Z}\left(r_p^2 - \frac{5}{3}\langle r^2\rangle_{\rm ch}\right)\mathbf{r}_p\ , \qquad (2)$$

Sensitivity factors for ^{19}F containing molecules

- The electron cloud around a ^{19}F nucleus in a diatomic metal-fluoride molecule is heavily polarized due to the ionic metal-fluorine bond, enhancing the molecule's sensitivity to ^{19}F NSM measurements.

Relativistic exact two-component coupled-cluster singles and doubles (X2C-CCSD)

- Reduce the storage requirement by an order of magnitude and computing time by a factor of four.
- Analytic X2C-CCSD gradient techniques help to avoid tedious and expensive numerical differentiation procedures.

Sensitivity factors for ^{19}F containing molecules

TABLE I. **Computed molecular sensitivity factors to the nuclear Schiff moment of ^{19}F for select molecules.** W_S is expressed in units of $\frac{e}{4\pi\epsilon_0 a_0^4} \approx 44.3\ h\ \mathrm{Hz}/(e\ \mathrm{fm}^3)$.

Molecule	Molecular state	$W_S\left(\frac{e}{4\pi\epsilon_0 a_0^4}\right)$
HfF^+	$a\,^3\Delta_1$	115
ThF^+	$X\,^3\Delta_1$	99
SrF	$X\,^2\Sigma^+$	52
BaF	$X\,^2\Sigma^+$	48
YbF	$X\,^2\Sigma^+$	59
TlF	$X\,^1\Sigma^+$	74
RaF	$X\,^2\Sigma^+$	47

- Of note, the magnitude of electron density close to the ^{19}F nucleus is significantly smaller than the nuclei of heavy metals in these molecules.

- Therefore, the ^{19}F NSM molecular sensitivity parameters are a few orders of magnitude smaller than those for the heavy atoms

EDM measurement and in HfF^+ its NSM interpretation

^{180}Hf, possesses a nuclear spin of zero ($I = 0$). Thus, the measurement is insensitive to nuclear-spin-dependent contributions from hafnium.

The HfF^+ EDM measurements were performed on the $a\,^3\Delta_1(v = 0, J = 1, F = 3/2, m_F = \pm 3/2)$ states, where v, J, and F correspond to the vibrational, rotational, and hyperfine quantum numbers, respectively, and m_F is the projection of F onto the quantization axis. This manifold was chosen to maximize the molecule's sensitivity to the electron's EDM. In the more precise of the two HfF^+ measurements [1], the energy splitting between EDM-sensitive molecular states was determined to be

$$hf = (-14.6 \pm 22.8_{\rm stat} \pm 6.9_{\rm syst})\ h\ \mu\text{Hz}, \tag{6}$$

hand side in Equation (1) evaluates to $|\langle \frac{\mathbf{I}\cdot\hat{n}}{I} \rangle| = 1/2$ in the $^3\Delta_1(v = 0, J = 1, F = 3/2, m_F = \pm 3/2)$ manifold [76]. Moreover, the experimental scheme measures the energy difference between the $m_F = +3/2$ and $m_F = -3/2$ states, in which the fluorine nuclear spin is oppositely oriented. A nonzero NSM shifts the energy of each state in opposite directions, so that the observed energy splitting corresponds to twice the NSM-induced shift in a single EDM-sensitive state, i.e.,

$$hf = 2|\Delta E_{\rm NSM}|. \tag{7}$$

$$hf = (-220\, g\bar{g}_0 - 160\, g\bar{g}_1 - 71\, g\bar{g}_2)\ h\ \text{Hz}. \tag{8}$$

EDM of the fluorine nucleus

$$h f_{\mathrm{EDM}} = 2\,|\mathbf{d}\cdot\boldsymbol{\mathcal{E}}_{\mathrm{unsc.}}|, \tag{9}$$

where $\mathbf{d}$ is the nuclear EDM and $\boldsymbol{\mathcal{E}}_{\mathrm{unsc.}}$ is the unscreened electric field seen by the ^{19}F atomic nucleus:

$$\boldsymbol{\mathcal{E}}_{\mathrm{unsc.}} = \frac{M}{M_{\mathrm{mol.}}}\frac{Q_{\mathrm{mol.}}}{Ze}\boldsymbol{\mathcal{E}}_{\mathrm{ext.}}, \tag{10}$$

where M is the mass of the ^{19}F atomic nucleus, $M_{\mathrm{mol.}}$ is the total mass of the molecular ion, $Q_{\mathrm{mol.}}$ is the net charge of the molecular ion, Z is the number of protons in the ^{19}F atomic nucleus, e is the elementary charge, and $\boldsymbol{\mathcal{E}}_{\mathrm{ext.}}$ is the applied external electric field.

The nuclear EDM of ^{19}F has been calculated using the NN-N^{3}LO + 3N$_{\mathrm{lnl}}$ interaction to be [48]:

$$d = (-0.018\,g\bar{g}_0 + 0.009\,g\bar{g}_1 - 0.023\,g\bar{g}_2)\ e\ \mathrm{fm}. \tag{11}$$

The coefficients in Equation (12) are much smaller than those in Equation (8). Hence, we shall neglect the effect of the nuclear EDM of ^{19}F in subsequent discussions.

In addition, we have computed the EDM of ^{19}F also with the NN-N^{4}LO + 3N$^*_{\mathrm{lnl}}$ and obtained results consistent with Equation (11) well within the 30% uncertainty quoted in Ref. [48].

At an applied electric field of 58 V/cm [1], Equations (9) and (11) translate to:

$$h f_{\mathrm{EDM}} = (0.53\,g\bar{g}_0 - 0.27\,g\bar{g}_1 + 0.68\,g\bar{g}_2)\ h\ \mathrm{Hz}. \tag{12}$$

TABLE II. **Upper bounds (90% confidence level) on $\mathcal{P},\mathcal{T}$-violating observables.** Definitions of $\bar{g}_{0,1,2}$ are provided in Equation (5). The bounds are derived using the $|S(^{19}\mathrm{F})|$ limit from Equation (13) and the coefficients in Equation (5). Each bound is calculated under the assumption that the corresponding observable is the sole contributor to the nuclear Schiff moment of ^{19}F. For the conversions, we use $g \approx 13.5$ [17]. These bounds are consistent with previous constraints [10].

Quantity	Limit
$\lvert\bar{g}_0\rvert$	1.6×10^{-8}
$\lvert\bar{g}_1\rvert$	2.2×10^{-8}
$\lvert\bar{g}_2\rvert$	4.8×10^{-8}

Discussion — Assuming that both the electron's EDM and the scalar–pseudoscalar nucleon–electron coupling are zero, we can place a bound on the NSM of ^{19}F:

$$|S(^{19}\mathrm{F})| < 9.0 \times 10^{-9}\ e\ \mathrm{fm}^3 \quad (90\%\ \text{confidence level}). \tag{13}$$

The conversion to a 90% confidence level follows the methodology described in Ref. [1].

If we further assume that each $\mathcal{P},\mathcal{T}$-violating observable in Equation (5) individually accounts for the entire NSM, we can derive bounds on these observables, as listed in Table II.

Using $\bar{g}_0 \approx -17.2 \times 10^{-3}\,\bar{\theta}$ [78] and $\bar{g}_1 \approx 3.4 \times 10^{-3}\,\bar{\theta}$ [78, 79], while neglecting the highly suppressed coupling $\bar{g}_2$ [80], we can also place a bound on the QCD θ term related to the strong $\mathcal{CP}$ problem [81, 82] :

$$|\bar{\theta}| < 1.1 \times 10^{-6} \quad (90\%\ \text{confidence level}). \tag{14}$$

of the NSM signal. As a result, the sensitivity of these molecules to the NSMs of heavy elements can be up to four orders of magnitude greater than to that of ^{19}F. Therefore, the contribution of the NSM of ^{19}F to the interpretation of EDM measurements in such systems is expected to be at the level of 10^{-4}. Although the ^{19}F NSM

Once remaining many-body challenges — such as effectively summing over all opposite-parity intermediate states coupled by the Schiff operator or treating nuclear deformation in the mass region beyond the doubly magic nucleus ^{208}Pb — are overcome, the NSMs of heavy, octupole-deformed nuclei are expected to come within reach of nuclear *ab initio* frameworks. Promising

Conclusion

- Present the first ab initio calculations of a nuclear Schiff moment(NSM), focusing on ^{19}F. By integrating (i) our nuclear structure calculations of the ^{19}F NSM, quantum chemistry analyses of molecular sensitivity to the NSM, and a detailed interpretation of the recent measurement of the electric dipole moment in HfF^{+}.
- From the first bound on the NSM of ^{19}F, we have derived the tightest limits yet on pion-nucleon-nucleon coupling constants using fully ab initio nuclear methods.
- This work demonstrates the power of ab initio approaches in connecting fundamental symmetries with experimental observables and paves the way for interpreting future precision measurements aimed at uncovering new sources of violations of fundamental symmetry in the nuclear sector.