BETTER ONUBB THROUGH BIOCHEMISTRY

SEARCHING FOR MAJORANA NEUTRINOS IN XENON GAS WITH SINGLE MOLECULE FLUORESCENCE IMAGING

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- Q: "What gives you hope that we could achieve anything like what you guys achieved in constructing the Standard Model today?"
- A. "The obvious answer is neutrino masses, which I think clearly take us beyond the standard model, and clearly represent something coming down from a very high energy scale."



Stephen Weinberg at the SLAC Summer Institute this year

 $-\frac{1}{2}\partial_{\nu}g^a_{\mu}\partial_{\nu}g^a_{\mu} - g_s f^{abc}\partial_{\mu}g^a_{\nu}g^b_{\mu}g^c_{\nu} - \frac{1}{4}g^2_s f^{abc}f^{ade}g^b_{\mu}g^c_{\nu}g^d_{\mu}g^e_{\nu} +$ $\tfrac{1}{2} i g_s^2 (\bar{q}_i^\sigma \gamma^\mu q_i^\sigma) g_\mu^a + \bar{G}^a \partial^2 G^a + g_s f^{abc} \partial_\mu \bar{G}^a G^b g_\mu^c - \partial_\nu W_\mu^+ \partial_\nu W_\mu^- M^2 W^+_{\mu} W^-_{\mu} - \frac{1}{2} \partial_{\nu} Z^0_{\mu} \partial_{\nu} Z^0_{\mu} - \frac{1}{2c_{-}^2} M^2 Z^0_{\mu} Z^0_{\mu} - \frac{1}{2} \partial_{\mu} A_{\nu} \partial_{\mu} A_{\nu} - \frac{1}{2} \partial_{\mu} H \partial_{\mu} H - \frac{1}{2} \partial_{\mu} H$ $\frac{1}{2}m_{h}^{2}H^{2}-\partial_{\mu}\phi^{+}\partial_{\mu}\phi^{-}-M^{2}\phi^{+}\bar{\phi^{-}}-\frac{1}{2}\partial_{\mu}\phi^{0}\partial_{\mu}\phi^{0}-\frac{1}{2c_{w}^{2}}M\phi^{0}\phi^{0}-\beta_{h}[\frac{2M^{2}}{a^{2}}+$ $\frac{2M}{a}H + \frac{1}{2}(H^2 + \phi^0\phi^0 + 2\phi^+\phi^-)] + \frac{2M^4}{a^2}\alpha_h - igc_w[\partial_\nu Z^0_\mu(W^+_\mu W^-_\nu \begin{array}{c} {}^{g} W_{\nu}^{+} W_{\mu}^{-}) - Z_{\nu}^{0} (W_{\mu}^{+} \partial_{\nu} W_{\mu}^{-} - W_{\mu}^{-} \partial_{\nu} W_{\mu}^{+}) + Z_{\mu}^{0} (W_{\nu}^{+} \partial_{\nu} W_{\mu}^{-} - W_{\nu}^{-} \partial_{\nu} W_{\mu}^{+})] - igs_{w} [\partial_{\nu} A_{\mu} (W_{\mu}^{+} W_{\nu}^{-} - W_{\nu}^{+} W_{\mu}^{-}) - A_{\nu} (W_{\mu}^{+} \partial_{\nu} W_{\mu}^{-} - W_{\nu}^{-} W_{\mu}^{-})] - igs_{w} [\partial_{\nu} A_{\mu} (W_{\mu}^{+} W_{\nu}^{-} - W_{\nu}^{+} W_{\mu}^{-}) - A_{\nu} (W_{\mu}^{+} \partial_{\nu} W_{\mu}^{-} - W_{\nu}^{-} W_{\mu}^{-})] - igs_{w} [\partial_{\nu} A_{\mu} (W_{\mu}^{+} W_{\nu}^{-} - W_{\nu}^{+} W_{\mu}^{-}) - A_{\nu} (W_{\mu}^{+} \partial_{\nu} W_{\mu}^{-} - W_{\nu}^{-} W_{\nu}^{-} W_{\nu}^{-})]$ $W^-_{\mu}\partial_{\nu}W^+_{\mu}) + A_{\mu}(W^+_{\nu}\partial_{\nu}W^-_{\mu} - W^-_{\nu}\partial_{\nu}W^+_{\mu})] - \frac{1}{2}g^2W^+_{\mu}W^-_{\mu}W^+_{\nu}W^-_{\nu} +$ $W^+_\nu W^-_\mu) - 2 A_\mu Z^0_\mu W^+_\nu W^-_\nu] - g \alpha [H^3 + H \phi^0 \phi^0 + 2 H \phi^+ \phi^-] \frac{1}{2}g^2\alpha_h[H^4 + (\phi^0)^4 + 4(\phi^+\phi^-)^2 + 4(\phi^0)^2\phi^+\phi^- + 4H^2\phi^+\phi^- + 2(\phi^0)^2H^2]$ $gMW^+_{\mu}W^-_{\mu}H - \frac{1}{2}g\frac{M}{c^2}Z^0_{\mu}Z^0_{\mu}H - \frac{1}{2}ig[W^+_{\mu}(\phi^0\partial_{\mu}\phi^- - \phi^-\partial_{\mu}\phi^0) W^{-}_{\mu}(\phi^{0}\partial_{\mu}\phi^{+}-\phi^{+}\partial_{\mu}\phi^{0})] + \frac{1}{2}g[W^{+}_{\mu}(H\partial_{\mu}\phi^{-}-\phi^{-}\partial_{\mu}H)-W^{-}_{\mu}(H\partial_{\mu}\phi^{+}-\phi^{-}\partial_{\mu}H)] + \frac{1}{2}g[W^{+}_{\mu}(H\partial_{\mu}\phi^{-}-\phi^{-}\partial_{\mu}H)] + \frac{1}{2}g[W^{+}_{\mu}(H\partial_{\mu}\phi$ $\phi^{+}\partial_{\mu}H)] + \frac{1}{2}g\frac{1}{c_{\mu}}(Z^{0}_{\mu}(H\partial_{\mu}\phi^{0} - \phi^{0}\partial_{\mu}H) - ig\frac{s^{2}_{\mu}}{c_{\mu}}MZ^{0}_{\mu}(W^{+}_{\mu}\phi^{-} - W^{-}_{\mu}\phi^{+}) +$
$$\begin{split} & igs_w MA_\mu (W^+_\mu \phi^- - W^-_\mu \phi^+) - ig \frac{1 - 2c_w^2}{2c_w} Z^0_\mu (\phi^+ \partial_\mu \phi^- - \phi^- \partial_\mu \phi^+) + \\ & igs_w A_\mu (\phi^+ \partial_\mu \phi^- - \phi^- \partial_\mu \phi^+) - \frac{1}{4} g^2 W^+_\mu W^-_\mu [H^2 + (\phi^0)^2 + 2\phi^+ \phi^-] - \end{split}$$
 $\frac{1}{4}g^{2}\frac{1}{c^{2}}Z_{\mu}^{0}Z_{\mu}^{0}[H^{2} + (\phi^{0})^{2} + 2(2s_{w}^{2} - 1)^{2}\phi^{+}\phi^{-}] - \frac{1}{2}g^{2}\frac{s_{w}^{2}}{c}Z_{\mu}^{0}\phi^{0}(W_{\mu}^{+}\phi^{-} +$ $W_{\mu}^{-}\phi^{+}) - \frac{1}{2}ig^{2}\frac{s_{w}^{2}}{c_{w}}Z_{\mu}^{0}H(W_{\mu}^{+}\phi^{-} - W_{\mu}^{-}\phi^{+}) + \frac{1}{2}g^{2}s_{w}A_{\mu}\phi^{0}(W_{\mu}^{+}\phi^{-} +$ $W^{-}_{\mu}\phi^{+}) + \frac{1}{2}ig^{2}s_{w}A_{\mu}H(W^{+}_{\mu}\phi^{-} - W^{-}_{\mu}\phi^{+}) - g^{2}\frac{s_{w}}{c_{w}}(2c_{w}^{2} - 1)Z^{0}_{\mu}A_{\mu}\phi^{+}\phi^{-} - W^{-}_{\mu}\phi^{+})$ $q^{1}s_{w}^{2}A_{\mu}A_{\mu}\phi^{+}\phi^{-}-\bar{e}^{\lambda}(\gamma\partial+m_{\lambda}^{\lambda})e^{\lambda}-\bar{\nu}^{\lambda}\gamma\partial\nu^{\lambda}-\bar{u}_{\lambda}^{\lambda}(\gamma\partial+m_{w}^{\lambda})u_{\lambda}^{\lambda} \overline{d}_i^{\lambda}(\gamma \partial + m_d^{\lambda})d_i^{\lambda} + igs_w A_{\mu}[-(\overline{e}^{\lambda}\gamma^{\mu}e^{\lambda}) + \frac{2}{2}(\overline{u}_i^{\lambda}\gamma^{\mu}u_i^{\lambda}) - \frac{1}{2}(\overline{d}_i^{\lambda}\gamma^{\mu}d_i^{\lambda})] +$ $\frac{ig}{4c_w}Z^0_{\mu}[(\bar{\nu}^{\lambda}\gamma^{\mu}(1+\gamma^5)\nu^{\lambda}) + (\bar{e}^{\lambda}\gamma^{\mu}(4s_w^2 - 1 - \gamma^5)e^{\lambda}) + (\bar{u}_j^{\lambda}\gamma^{\mu}(\frac{4}{3}s_w^2 - 1 - \gamma^5)e^{\lambda}) + (\bar{u}_j^{\lambda}\gamma^{\mu}(\frac{4}{3}s_w^2 - 1 - \gamma^5)e^{\lambda}) + (\bar{u}_j^{\lambda}\gamma^{\mu}(1+\gamma^5)\nu^{\lambda}) + (\bar{e}^{\lambda}\gamma^{\mu}(1+\gamma^5)\nu^{\lambda}) + (\bar{e}^{\lambda}\gamma^{\mu}(1+\gamma^5)e^{\lambda}) + (\bar{e}^{\lambda}\gamma^{\mu}(1+\gamma^5)e^{$ $(1 - \gamma^5)u_j^{\lambda}) + (\bar{d}_j^{\lambda}\gamma^{\mu}(1 - \frac{8}{3}s_w^2 - \gamma^5)d_j^{\lambda})] + \frac{ig}{2\sqrt{2}}W_{\mu}^+[(\bar{\nu}^{\lambda}\gamma^{\mu}(1 + \gamma^5)a_j^{\lambda}) + \bar{\nu}^{\lambda})$ $(\bar{u}_{j}^{\lambda}\gamma^{\mu}(1+\gamma^{5})C_{\lambda\kappa}d_{j}^{\kappa})] + \frac{ig}{2\sqrt{2}}W_{\mu}^{-}[(\bar{e}^{\lambda}\gamma^{\mu}(1+\gamma^{5})\nu^{\lambda}) + (\bar{d}_{j}^{\kappa}C_{\lambda\kappa}^{\dagger}\gamma^{\mu}(1+\gamma^{5})\nu^{\lambda})]$ $\gamma^{5}(u_{i}^{\lambda})] + \frac{ig}{2\sqrt{2}} \frac{m_{i}^{\lambda}}{M} [-\phi^{+}(\bar{\nu}^{\lambda}(1-\gamma^{5})e^{\lambda}) + \phi^{-}(\bar{e}^{\lambda}(1+\gamma^{5})\nu^{\lambda})] \frac{g}{2}\frac{m_{\epsilon}^{\lambda}}{M}[H(\bar{e}^{\lambda}e^{\lambda}) + i\phi^{0}(\bar{e}^{\lambda}\gamma^{5}e^{\lambda})] + \frac{ig}{2M\sqrt{2}}\phi^{+}[-m_{d}^{\kappa}(\bar{u}_{j}^{\lambda}C_{\lambda\kappa}(1-\gamma^{5})d_{j}^{\kappa}) +$ $m_u^{\lambda}(\bar{u}_j^{\lambda}C_{\lambda\kappa}(1+\gamma^5)d_j^{\kappa}] + \frac{ig}{2M\sqrt{2}}\phi^{-}[m_d^{\lambda}(\bar{d}_j^{\lambda}C_{\lambda\kappa}^{\dagger}(1+\gamma^5)u_j^{\kappa}) - m_u^{\kappa}(\bar{d}_j^{\lambda}C_{\lambda\kappa}^{\dagger}(1-\gamma^5)u_j^{\kappa})] + \frac{ig}{2M\sqrt{2}}\phi^{-}[m_d^{\lambda}(\bar{d}_j^{\lambda}C_{\lambda\kappa}^{\dagger}(1+\gamma^5)u_j^{\kappa}) - m_u^{\kappa}(\bar{d}_j^{\lambda}C_{\lambda\kappa}^{\dagger}(1+\gamma^5)u_j^{\kappa})] + \frac{ig}{2M\sqrt{2}}\phi^{-}[m_d^{\lambda}(\bar{d}_j^{\lambda}C_{\lambda\kappa}^{\dagger}(1+\gamma^5)u_j^{\kappa})] + \frac{ig}{2M\sqrt{2}}\phi^{-}[m_d^{\lambda}(\bar{d}_j^{\lambda}C_{\lambda\kappa}^{\dagger}(1+\gamma^5)u_j^{\kappa})] + \frac{ig}{2M\sqrt{2}}\phi^{-}[m_d^{\lambda}(1+\gamma^5)u_j^{\kappa}) - \frac{ig}{2M\sqrt{2}}\phi^{-}[m_d^{\lambda}(1+\gamma^5)u_j^{\kappa}] + \frac{ig}{2M\sqrt{2}}\phi^{-}[m_d^{\lambda}(1+\gamma^5)u_j^{\kappa})] + \frac{ig}{2M\sqrt{2}}\phi^{-}[m_d^{\lambda}(1+\gamma^5)u_j^{\kappa})] + \frac{ig}{2M\sqrt{2}$ $\gamma^5 u_j^\kappa \left[-\frac{g}{2} \frac{m_u^\lambda}{M} H(\bar{u}_j^\lambda u_j^\lambda) - \frac{g}{2} \frac{m_d^\lambda}{M} H(\bar{d}_j^\lambda d_j^\lambda) + \frac{ig}{2} \frac{m_u^\lambda}{M} \phi^0(\bar{u}_j^\lambda \gamma^5 u_j^\lambda) - \right]$ $\frac{ig}{2}\frac{m_d^{\lambda}}{M}\phi^0(\bar{d}_j^{\lambda}\gamma^5 d_j^{\lambda}) + \bar{X}^+(\partial^2 - M^2)X^+ + \bar{X}^-(\partial^2 - M^2)X^- + \bar{X}^0(\partial^2 - M^2$ $\frac{M^2}{c^2}$ $X^0 + \bar{Y}\partial^2 Y + igc_w W^+_\mu (\partial_\mu \bar{X}^0 X^- - \partial_\mu \bar{X}^+ X^0) + igs_w W^+_\mu (\partial_\mu \bar{Y} X^- \partial_{\mu}\bar{X}^{+}Y) + igc_{w}W^{-}_{\mu}(\partial_{\mu}\bar{X}^{-}X^{0} - \partial_{\mu}\bar{X}^{0}X^{+}) + igs_{w}W^{-}_{\mu}(\partial_{\mu}\bar{X}^{-}Y - \partial_{\mu}\bar{X}^{-}) +$ $\partial_{\mu}\bar{Y}X^{+}) + igc_{w}Z^{0}_{\mu}(\partial_{\mu}\bar{X}^{+}X^{+} - \partial_{\mu}\bar{X}^{-}X^{-}) + igs_{w}A_{\mu}(\partial_{\mu}\bar{X}^{+}X^{+} - \partial_{\mu}\bar{X}^{-}X^{-}) + igs_{w}A_{\mu}(\partial_{\mu}\bar{X}^{+}X^{+}) + igs_{w$ $\partial_{\mu}\bar{X}^{-}X^{-}) - \frac{1}{2}gM[\bar{X}^{+}X^{+}H + \bar{X}^{-}X^{-}H + \frac{1}{c^{2}}\bar{X}^{0}X^{0}H] +$ $\frac{1-2c_w^2}{2c_w}igM[\bar{X}^+X^0\phi^+ - \bar{X}^-X^0\phi^-] + \frac{1}{2c_w}igM[\bar{X}^0X^-\phi^+ - \bar{X}^0X^+\phi^-] +$ $igMs_w[\bar{X}^0X^-\phi^+ - \bar{X}^0X^+\phi^-] + \frac{1}{2}igM[\bar{X}^+X^+\phi^0 - \bar{X}^-X^-\phi^0]$

← The standard model Lagrangian we all know and love

Write down all terms that are:

1) Consistent with the symmetries groups of the SM

Gauge invariance: $SU(3) \times SU(2)_L \times U(1)_Y$

+ Lorentz invariance

2) Renormalizible

If SM is a low energy effective theory:





Seems likely (LHC) Maybe? (GUT scale) If SM is a low energy effective theory:

$$L = L_{SM} + \frac{1}{E_{new}}L_1 + \frac{1}{E_{new}^2}L_2 + \dots$$

 The only dimension-5 operator one can add obeying SM gauge symmetry:

$$\frac{L_1}{E_{new}} = y_{ij} \frac{\nu^i H \nu^j H}{E_{new}}$$

Weinberg 1979.

- This term does an important thing it makes neutrinos Majorana particles, with mass suppressed by the new physics scale.
- And it makes the theory non-renormalizible implying there must be something else at high scale (see also: Seasaw)

The Weirdness of Majorana Fermions



Behaves like matter

Behaves like antimatter

Double-Beta Decay

A rare radioactive process, energetically allowed for some even-even nuclei where $m_{Z+1} > m_Z > m_{Z+2}$

• $(Z,A) \to (Z+2,A) + e_1^{-} + v_1^{-} + e_2^{-} + v_2^{-}$

allowed $\beta\beta$ ferevel in \overline{v}_{e}

Discovered in 1987 in ⁸²Se and now seen in multiple isotopes



Types of double beta decay



A known standard model process and an important calibration tool

$$T_{\frac{1}{2}} \approx 10^{19-21} yrs.$$

Final state: e⁻ e⁻ v_e v_e

Observation would prove that the neutrino is a Majorana fermion

$$T_{\frac{1}{2}} \approx$$
 ????

Final state: e⁻ e⁻





1. This formula \rightarrow

$$\frac{1}{T_{\frac{1}{2}}} = \boldsymbol{G} \times \left\| \mathbf{M} \right\|^2 \times \boldsymbol{m}_{\overline{\boldsymbol{v}}}^2$$



1. This formula \rightarrow

$$\frac{1}{T_{\frac{1}{2}}} = \boldsymbol{G} \times \left\| \boldsymbol{M} \right\|^2 \times \boldsymbol{m}_{\bar{\boldsymbol{v}}}^2$$

← 2. Nuclear matrix elements



3. Effective nu mass ^





Cute story, but...



- Strength of weak interaction is quenched in nuclear medium
 - Rate depends on 4th power of g_A
 - Nobody really knows where the "NH" and "IH" bands are.
- All those plots assume light Majorana neutrino exchange mechanism.
 - Motivated by seesaw models.
 - But Majorana neutrinos imply generically new high-scale physics, and generically new physics can produce generic 0nubb rates.

Warning: don't stick to $m_{\beta\beta}$ metric, just go on with $T_{1/2}$! Variety of $0\nu\beta\beta$ mechanisms:













$0\nu\beta\beta$ from any mechanism \rightarrow Majorana nature of ν would be established anyway

Slide from <u>The Mid and Long Term Future of Neutrinoless Double Beta Decay</u>, Andrea Giuliani, Neutrinno2018, https://doi.org/10.5281/zenodo.1286915 A robust observation of Onubb would tell us 6 things about nature before breakfast:

1) Lepton number conservation is violated.

2) Massive fermions exist that are neither matter or antimatter but something else (Majorana fermions)

3) The SM with the Majorana term is non-renomalizible \rightarrow SM is definitely a low energy effective theory.

4) There are other mass generating mechanisms in nature beyond the Higgs mechanism.

5) Like G_F tells us the weak scale and ultimately leads to W and Z mass predictions, m_v tells us the next scale.

6) Majorana neutrinos are a prediction of the theory of Leptogenesis that may generate observed matter/anti-matter asymmetry of the Universe (given enough CPV – see also: DUNE)

So how about we all agree to:

Be as sensitive as possible

(get out logarithmically into unexplored parameter space)

Build experiments that can make discoveries, not just set limits

(well understood detectors with clear, positive signal criteria)

The ideal experiment:



• MANDATORY:

 Resolution better than ~2% FWHM to fully reject twoneutrino mode

Then just watch and wait...

The non-ideal experiment:



• MANDATORY:

 Resolution better than ~2% FWHM to fully reject twoneutrino mode

• Ideally:

 Would have zero other backgrounds

Then just watch and wait...





Neutrinoless Double Beta Decay Searches











100kg-class experiments:



Methods to achieve lower background

- Reject 2vββ tail:
 - Energy resolution is only handle
 - ~2% FWHM reaches 0.1 ct ton yr.



For cartoon purposes only

Reject radioactive backgrounds Typically ²¹⁴Bi, ²⁰⁸Th from uranium

and thorium chains respectively:

- Shielding / radiopurity
- Energy resolution
- Topological signature
- Daughter tag



nEXO (left) and NEXT-100 (right) background models

The NEXT Program



Sequence of HPGXe TPCs, focused on achieving big, very low background xenon 0vββ detector



Full underground technology demonstrator @10kg scale









Energy Plane



Tracking Plane



Field Cage



Anode



The Next White (NEW) Detector F. Monrabal et. al. arXiv:1804.02409

The NEXT Program



 Sequence of HPGXe experiments, focused on achieving big, very low background xenon 0vββ detector

→ NEXT-DBDM

- → NEXT-DEMO
- \rightarrow NEXT-NEW

→ NEXT-100

 \rightarrow NEXT-XXX



100 kg scale neutrinoless double beta decay search and background-study for ton-scale

NEXT-100 cathode and electroluminescence regions built and tested at UTA





Why Xenon Gas?

1) Energy resolution

2) Topology

3) Practicality at ton-scale

Why Xenon Gas?

1) Energy resolution

Fluctuation-less EL gain and low Fano factor produces resolution comparable with solid-state technologies in a monolithic TPC experiment

2) Topology

3) Practicality at ton-scale

Bolotnikov and Ramsey. "<u>The</u> <u>spectroscopic properties of</u> <u>high-pressure xenon</u>."NIM A 396.3 (1997): 360-370



Initial results on energy resolution of the NEXT-White detector J. Renner et al, arXiv 1808:01804



Why Xenon Gas?

1) Energy resolution

Fluctuation-less EL gain produces resolution comparable with solid-state technologies in a monolithic TPC experiment

2) Topology

Lower density allows powerful single-vs-multi electron and single-vs-multi-site topological background rejection

3) Practicality at ton-scale




Why Xenon Gas?

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3) Practicality at ton-scale

Reliance on active background rejection rather than self shielding means program uses isotope efficiently and can be phased **NEXT-XXX:** 202?

NEXT-NEW

66 cm

Running





Self-shielding based (KamlandZen, nEXO, etc)

Several tons of isotope for each clean ton



Active background rejection based (CUORE, MAJORANA/GERDA, NEXT, etc)

1 ton of isotope for each clean ton.



Phase-able deployment possible

Low-risk, reliable, cost effective approach to hitting background targets

1.7T



NEXT-100 in 2019 will be comfortably world leading in xenon, and competitive with world leaders in other isotopes.



BUT WORLD-LEADING IS NOT ENOUGH!

Barium Tagging

- Barium ion is only produced in a true ββ decay, not in any other radioactive event.
- Identification of Ba ion plus ~1% FWHM energy measurement would give a background-free experiment.
- Is it plausible to detect an individual barium ion or atom in a ton of material?





Barium tagging for 0nubb has been actively explored in liquid and gas xenon for >15 years, with the holy grail is a scalable single ion sensitive technology.



Basics - Barium Atoms and Ions

- Barium is born in a high charge state as emerging beta electrons disrupt the atom
- Quickly captures electrons from xenon to reach the Ba⁺⁺ state
- In gas, it ~stops there. In liquid, further recombination happens.



Liquid – Some distribution





Ionic Charge State in Liquid and Gas



Charge States

- "Best guess" assumptions:
 - Ba++ has 2x larger Onsager radius than Ba+, so expect 4x larger capture cross section for recombination.
 - In double beta decay, two emerging tracks at nucleus, so 2x recombination of single decay.
- Guesstimate Ba charged fractions in double beta decay →



Q: How do you make Ba⁺⁺ shine?



Concept to adapt SMFI for Ba tagging: D.R. Nygren, J.Phys.Conf.Ser. 650 (2015) no.1, 012002

SMFI:

 A non-fluorescent molecule becomes fluorescent (or vice versa) upon chelation with an incident ion.



Calcium and barium are congeners – many dyes developed for calcium are also expected to respond to barium

SMFI is a technique from biochemistry with demonstrated single-ion resolution.



← Rhod-2 sensing Ca⁺⁺ production in rat astrocyte cells

J Cell Biol 145, 795 (1999).

Single molecule tracking using SMFI is the basis of super-resolution microscopy→

These methods won the Nobel Prize in chemistry in 2014.

J Microsc. 2011 Apr;242(1):46-54





← First dabbling developed a bespoke fluorescence sensor to study barium production at the end of a fiber.

<u>Single molecule fluorescence imaging</u> <u>as a technique for barium tagging in</u> <u>neutrinoless double beta decay</u> Jones, McDonald, Nygren, JINST (2016) 11 P12011

We find strong fluorescence from Fluo3 and Fluo4 under chelation with Ba⁺⁺ ions →



Microscope objectives:



Goal in life: Do its darnedest to turn point sources into parallel rays and vice versa.













Fluorescence microscopy

51

Single Ba⁺⁺ TIRF images from our lab at UTA



 ← This image shows a weak solution of barium perchlorate salt on our sensor.

Each spot is a **single barium ion**.

Brighter spots are near the TIRF surface, dimmer ones are deeper in the sample.

In a xenon detector, dye deposited as a monolayer and only brightest spots at constant depth expected.



This "step" is how you know it is exactly one ion.



Single ions barium resolved with 2nm super-resolution and 12.9 sigma stat. significance.

Phys.Rev.Lett. 120 (2018) no.13, 132504

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Physics News and Commentary

Barium Ion Detector for Next-Generation Neutrino Studies

March 26, 2018

A device that can detect individual barium ions could be the heart of an experiment that takes the next step toward probing the nature of the neutrino.

Focus story on: A.D. McDonald et al. (NEXT Collaboration) Phys. Rev. Lett. 120, 132504 (2018)

First demonstration of single Ba++ ion resolution.

Next steps: Making it work in gas

- 1. Barium ion test beam
- 2. Barium drift characterization
- 3. Dry phase microscopy
- 4. Ion concentration to sensors
- 5. Dry SMFI molecule design
- 6. Combine into a working sensor for NEXT prototype





The barium beam

- The next major step is to test barium sensing dyes in HPGXe environment
- Expect better performance than in solution from both energetics and reactivity considerations





Barium or barium coated needle goes here

We have developed a custom electroplating method to deposit a stable barium-rich coating onto copper for spark source from methanol.

Removes difficulty of barium metal handling.



Bare copper

Barium electroplated copper



Barium mobility in gas – in theory:



Mobility and Clustering of Barium Ions and Dications in High Pressure Xenon Gas E. Bainglass, B.J. P. Jones, et. al. Phys.Rev. A97 (2018) no.6, 062509

Excellent agreement with data for Ba+

For Ba++ things get more complicated.



Calculated Ba++ clusters:



Bigger clusters more similar to each other, so less pressure dependence in Ba++ than Ba+

Isotopic composition changes scattering kinematics, so %-level differences with enriched xenon

We will test this with experimental data soon!

The ion beam is coming...





Gated Drift Region

20cm uniform drift region that utilized Bradbury-Nielsen gates. These gates allow for the inital ion cloud to be chopped in order to minimize the space charge effect on the ions drift

Readout Plane

A readout chamber that allows the use of sensitive eletrical amplifier or optical readout. The ions are guided here via an eletric field.

Ion Source

A needle and ring electrode that is adjustable allowing for an adjustable spark gap to acomadate Various pulse and pressure conditions.

Dry Microscopy

- To remove microscope oil (incompatible with HPGXe) we need to deliver excitation transversely.
- This is achieved through prism TIRFdecouples the motion of the objective and the TIRF source.
- We are building up a prism TIRF array at UTA for operation in gas





Dry Phase Receptor

Deprotonation of carboxylic acids is required to accept the ion – we observe the characteristic pH dependence of this in solution



It is unclear if deprotonation will occur in solid phase but we suspect perhaps not. This motivated us to start building "dry-taylored" molecules even before we have a dry system to test in.



Fluo-3 may not be ideal for HPGXe, since fluorescein dye is not bright in dry phase.

But pyrene works. We can resolve single molecules of it too.



The Dream Molecule?

Tethered pyrene substituted monoazocryptand (tPSMA)

Our first batch is being synthesized right now by Foss lab at UTA.



Monoazocryptand (hyper Ba⁺⁺ specific) Diner, C., Scott, D. E., Tykwinski, R. R., Gray, M. R., & Stryker, J. M. Scalable, Chromatography-Free Synthesis of Alkyl-Tethered Pyrene-Based Materials. Application to First-Generation "Archipelago Model" Asphaltene Compounds. *J. Org. Chem.* **2015**, *80*(3), 1719–1726. Synthesis of PSMA and its relatives

The story so far...

First batch of custom dry fluorophores coming off production line now.

Watch this space!



Implementation in NEXT

- The NEXT collaboration is exploring implementation of a prototype barium tagging sensor in a near-future phase of NEXT.
- Our R&D plan aims to converge on an end-to-end barium tagging scheme by 2022-2023. Optimistic, but looks possible from where we stand now.
- A ton-scale barium tagging HPGXeTPC may be what we need to uncover the Majorana nature of the neutrino, and open the window to the next energy scale.



THIS QUESTION OF NEUTRINO MASS IS TOO IMPORTANT NOT TO ANSWER, OR TO ANSWER AMBIGUOUSLY.



Thanks! on behalf of...


Thanks!



Superposed fields:

RF creates effective potential that levitates ions without neutralization Surfing field sweeps ions to center,





MAC Synthesis: cis-crown ether



Orientation of the Pyrene Moiety



•Langmuir, **2008**, 24, 5140-5145

168 SINGLE MOLECULE FLUORESCENCE SPECTROSCOPY

Fluorophore	λ_{ex}^{1p}	λ^{1p}_{em}	QY	<i>E</i>	SS	τ_{f}	λ_{ex}^{2p}	λ_{em}^{2p}	Reference
	(nm)	(nm)		(cm ⁻ 'M ⁻ ')	(nm)	(ns)	(nm)	(nm)	
FITC	495	520	0.7	73,000	25	—	947	530	[87–89]
FAM	495	520	0.7	83,000	25	_			[88]
TMR	554	585	0.2-0.5	95,000	31	2.1	849	570	[5,90,91]
R6G	530	556		105,000	26				[92]
Cy2	489	506			17		905	520	[87,93]
Cy3	550	570	0.14	150,000	20	~1	1032	578	[3,87,90]
Cy5	650	670	0.15	250,000	20	~1			[3,5,90]
Cy5.5	675	694		250,000	19	_			[3]
Cy7	743	767	0.02	250,000	24	~0.8			[3,90,94]
ECFP	458	472	0.4	26,000	14	_	_	_	[94]
EGFP	395,470	509	0.8	30,000	39	3.2			[5,90,94]
EYFP	514	527	0.6	84,000	13	3.7		_	[90,94]
DsRed	532	582	0.29	22,500	50	2.8	_	_	[90]
Bodipy Fl	504	510	_	70,000	6	_	920	526	[87,88]
Bodipy R6G	528	547		70,000	19	_		_	[88]
AF488	495	520	0.5-0.9	80,000	25	_	985	530	[5,87]
AF546	554	570	_	112,000	16	_	1028	582	[87,95]
AF555	555	565		150,000	10				[3]
AF594	590	617		92,000	27		1074	619	[87,95]
AF633	632	647		100,000	15	3.2			[3,90]

Table 4.1 Photophysical properties of some common dyes with potential for single molecule fluorescence studies



Fluoroscein: FITC + FAM



Rhodamine: TMR, R6G



Handbook of Single Molecule Fluorescence, Gell, C. Brockwell, D. Smith, A. OUP Oxford, 2006, New York p. 168-9.

Alternative Fluorophores





Ando, Hiruta, Citterio, Suzuki Analyst, 2009, 134, 2314-2319

Hiruta, Sato, Takahashi, Kubobuchi, Shichi, Citterio, Suzuki RSC Adv. 2013, 3, 6499-6506

The basic SMFI method:

 A non-fluorescent molecule becomes fluorescent (or vice versa) upon chelation with an incident ion.



 Calcium and barium are congeners – many dyes developed for calcium are also expected to respond to barium













The key to the tagging behavour of PSMA is a carefully placed lone pair of electrons on the nitrogen atom.

The PSMA magic:





The PSMA magic:









Back in the ground state with no fluorescence!











Fluorescence is switched on only when barium ion is present

The basic SMFI method:

 A non-fluorescent molecule becomes fluorescent (or vice versa) upon chelation with an incident ion.



 Calcium and barium are congeners – many dyes developed for calcium are also expected to respond to barium

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The key to the tagging behavour of PSMA is a carefully placed lone pair of electrons on the nitrogen atom.

The PSMA magic:





The PSMA magic:









Back in the ground state with no fluorescence!











Fluorescence is switched on only when barium ion is present

A scaling challenge: EL amplification

 Ongoing work at UTA to develop large, stable, uniform EL amplification plane for NEXT-100 (D=1.2 m) and NEXT-XXX (D~1.5m)



High Voltage Insulation and Gas Absorption of Polymers in High Pressure Argon and Xenon Gases arXiv:1804.04116. L.Rogers et. al.



PROUDLY SUPPORTED BY:



Energy loss through ionization



Ionization

A well defined energy fraction is converted into ionization electrons

"Intrinsic" energy resolution achievable by measuring ionization at 2400MeV is around 0.3% at $Q_{\beta\beta}$

Fano Factor = 0.15
At high densities...

(gas >50 bar and liquid)



At high densities, ionization charge is lost to recombination

The recombination process is random, and this introduces fluctuations \rightarrow intrinsic resolution is degraded *(ionization no longer carries a well known fraction of event energy)*

At high densities...

(gas >50 bar and liquid)



fluctuations. This is what liquid experiments do.

In gas @15 bar, no recombination and so no recombination fluctuations.



Caveat:

- All the liquid lines are E-field dependent

- Gas has minimal recombination so ~no E-field dependence

Amplifying the charge

- In high pressure gas, measuring ionization charge **alone** gives excellent energy resolution (0.3%) **in principle.**
- Now the challenge is to amplify it without introducing fluctuations.
- Use electroluminescent gain mechanism:



Electrons get enough energy to ionize as well as excite Xe: → big fluctuations in photon yield



Only enough energy to excite Xe → small fluctuations in photon yield



That this can happen suggests two ions may trap in a single pore in PVA matrix (v. rare)

Barium ion mobility in gas

 Measurements from Medina's PhD thesis illustrate the importance of molecular ion formation.

 $Ba^+ + Xe + Xe \longleftrightarrow BaXe^+ + Xe$

- Never measured in Ba⁺⁺ to our knowledge
- And not measured above 1 bar to our knowledge either

From "Mobility and fluorescence of barium ions in xenon gas for the EXO experiment" – Julio Cesar Benitez Madina, PhD thesis, Colorado State University



DFT vs coupled clusters

- Past published calcs used coupled cluster theory – good for bare ion ONLY.
- We calculate cluster distributions and cross sections using density functional theory then evaluate mobility.
- DFT is not expected to be as accurate. But too many atoms for coupled cluster method.
- We benchmark our DFT

 ion mobility
 calculations for bare
 ions against McGuirk,
 and experimentally
 extracted data for BaXe
 system.



%-level agreement

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Comparison of potentials

Comparison of mobilities

Ba++ clusters much more



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NEXT-100 projected background index performance



← Approximately
 Background free @
 100kg-scale

World-leading in xenon by an order of magnitude, but still ~5-7 cts/yr at ton scale

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²²Na calibration of NEXT-NEW

- Preliminary results:
- 6.75% FWHM (0.74% at QBB) resolution for x-rays (29.6 keV).
- 2.35% FWHM (1.07% at Q_{BB}) resolution for 511 keV γ.
- Continuing improvements from improved analysis methods and detector stability.





