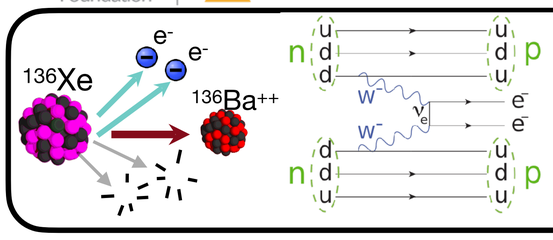
BOLD: strategies to produce and detect single Ba^{2+} ions using molecular indicators in the NEXT 0νββ decay experiment

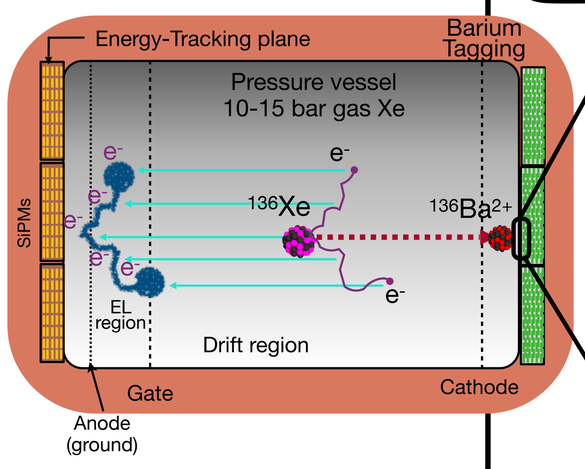
Pablo Herrero Gómez on behalf of the NEXT collaboration.



The NEXT collaboration seeks the neutrinoless double beta (0νββ) decay $^{136}Xe \rightarrow {}^{136}Ba^{2+} + 2e^-$, as an unambiguous proof of the Majorana nature of neutrinos. No other radioactive decay produces such ion in coincidence with two electrons. Thus, detection of the daughter atom of the decay, Ba^{2+}, would remove all reducible background. This can be done through Single Molecule Fluorescence Imaging of chemo-sensors designed to selectively capture Ba^{2+}. We present three different families of molecular indicators which produce different types of fluorescence signals.

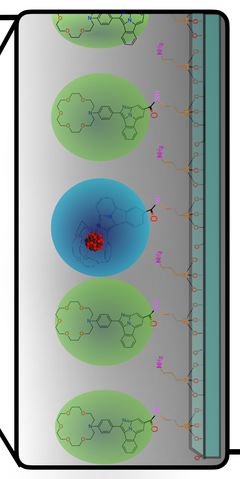
1 Ba^{2+} tagging sensor: the concept

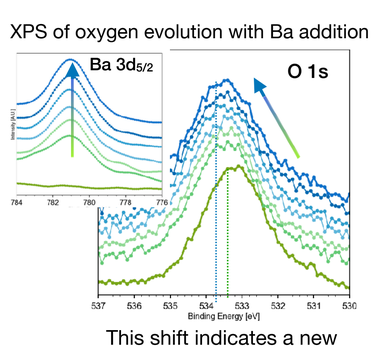
1. Discovery of 0νββ decay of ^{136}Xe would prove the Majorana nature of neutrinos and help extending the Standard Model.
2. NEXT reconstructs the shape and energy of a track left by $2e^-$ in the decay of ^{136}Xe.
3. Ba^{2+} drifts to the cathode where a monolayer of organic molecules captures it and emits a fluorescence signal.
4. Detection of Ba^{2+} in delayed coincidence with the electron track has an associated virtually **zero** background [1].
5. The challenge is finding **a single Ba^{2+} ion** in a chamber with > 1 ton of Xe and on an area of ~1 m^2.



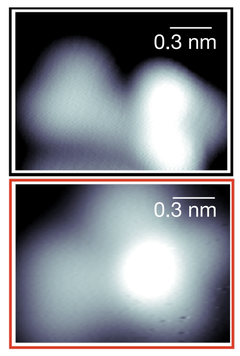
2 Single-Ion Molecular Indicators on surfaces

1. The sensor is formed by a monolayer of organic molecules that yield a fluorescent signal when binding specifically with Ba^{2+} [2].
2. Interaction with Ba^{2+} (chelation) produces structural and chemical changes in the molecule that can be measured by surface science techniques like XPS and STM/STS [3].

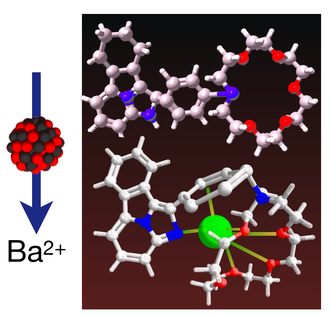




This shift indicates a new chemical bond appeared



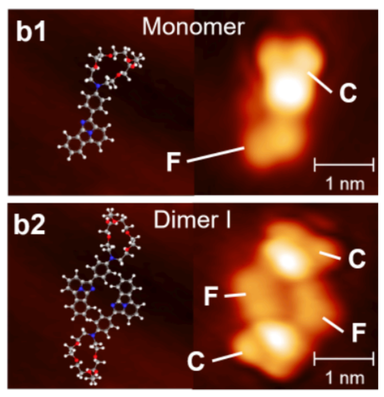
Tunnel microscope images showing rearrangement of molecular orbitals.



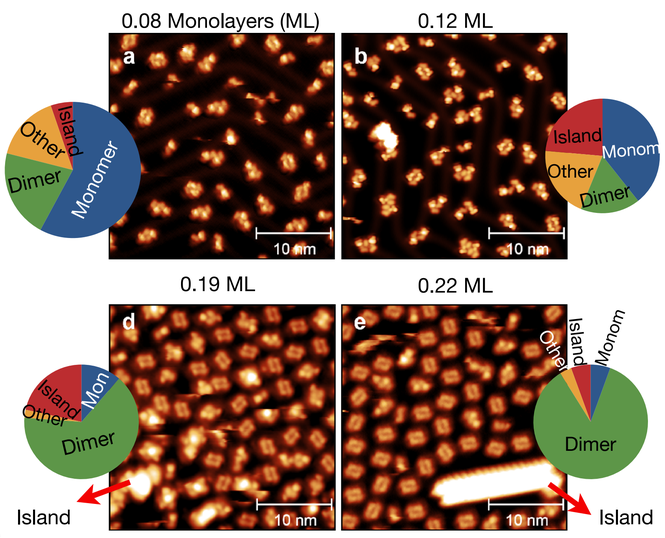
Sub-monolayer sensor model (DFT calculations)

Three sensing strategies

3 Arrangement on surfaces



3. The molecules aggregate on surfaces forming **monomers** (b1), **dimers** (b2) or **islands** [7].
4. The most abundant type of aggregation changes with the coverage of the surface:



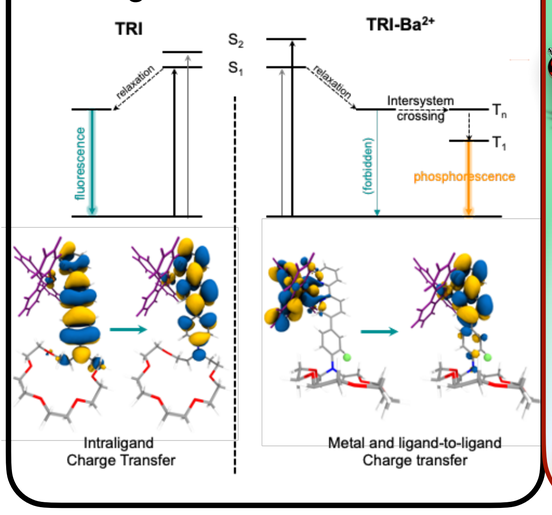
4 Fluorescence vs Phosphorescence

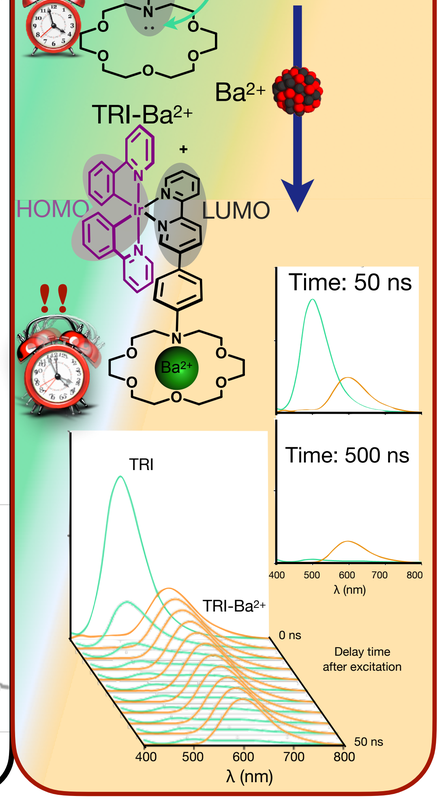
Time-resolved indicators not only produce a bicolor signal but also different time signatures [7].

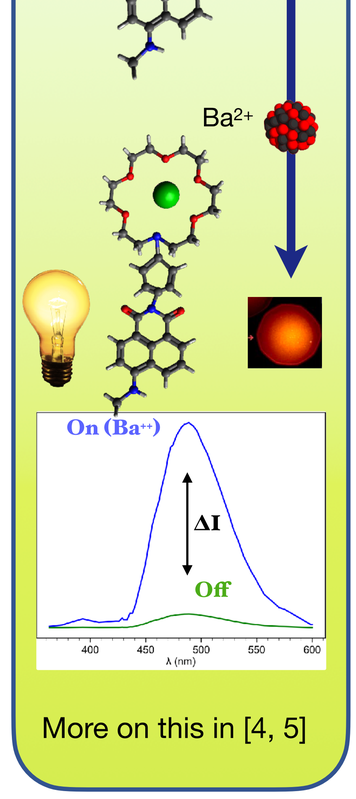
The free molecule emits fluorescence from a **singlet** excited state.

The chelated molecule can emit phosphorescence by intersystem crossing to a **triplet** excited state.

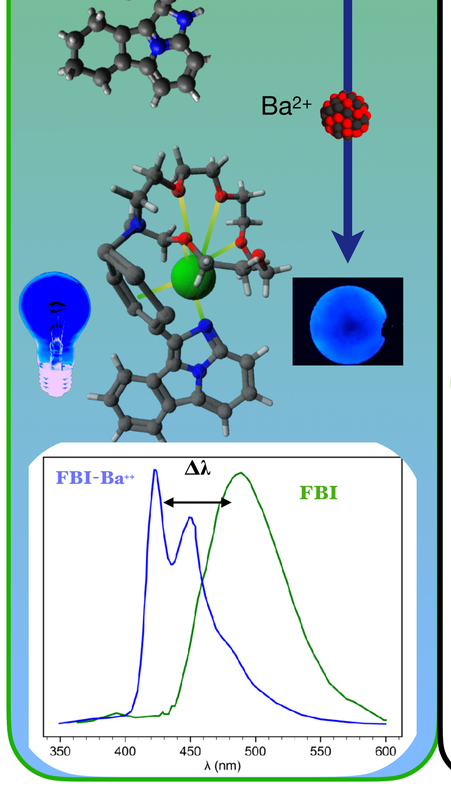
Thus, chelated molecules **keep emitting** after unchelated faded off.





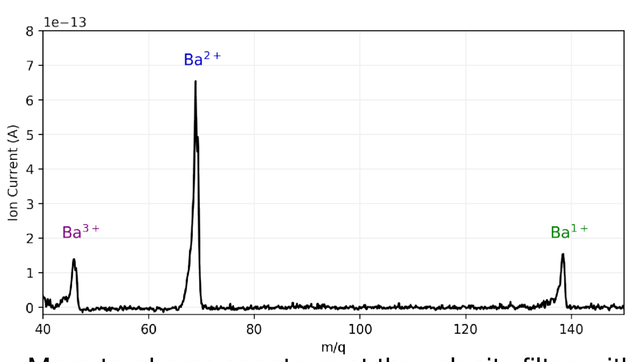


More on this in [4, 5]



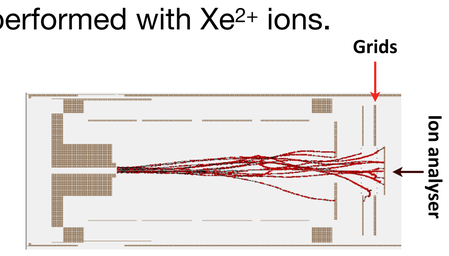
5 Barium beam emulating NEXT conditions

1. Sources of Ba^{2+} consist in evaporating Ba as salt [3] or metal and ionising it [6].
2. The source at Ben Gurion University includes a velocity filter, a direction steerer into a thermalisation chamber. The atom reaches the surface of the sample with **low** energy.
3. Different cations are produced in the evaporation. Ba^{2+} is filtered by its m/q ratio.

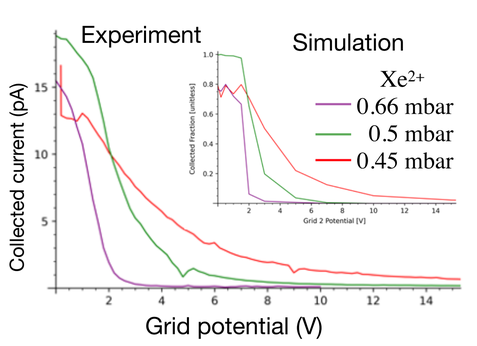


Mass to-charge spectrum at the velocity filter, with the dominant ions, Ba^{1+}, Ba^{2+} and Ba^{3+} at 138, 69 and 46, respectively.

4. **Characterization** of the beam was performed with Xe^{2+} ions.

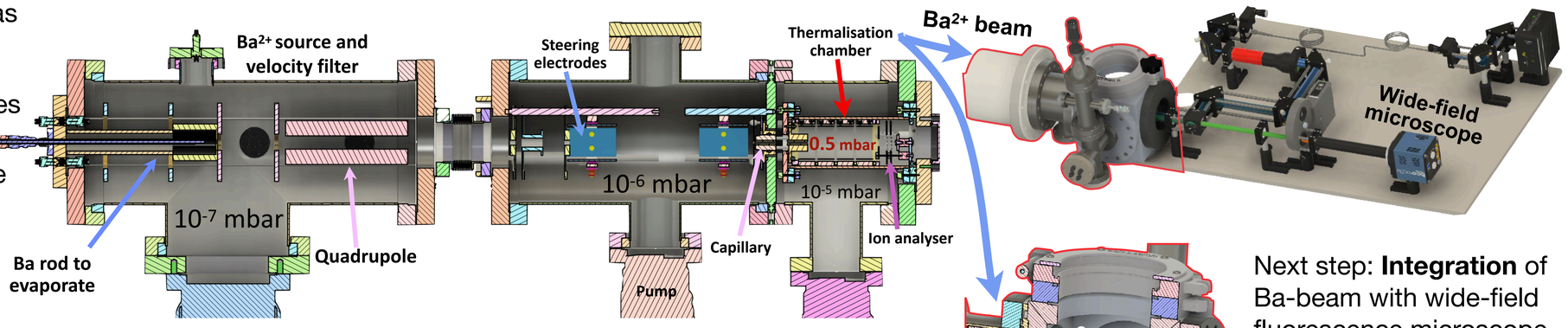


Thermalization chamber simulation: ions passing through the capillary can reach the analyser



Good agreement between measurements and SIMION simulations [7].

6 Outlook: *in-situ* detection of chelation



Next step: **Integration** of Ba-beam with wide-field fluorescence microscope that will allow for *in situ* detection of **single Ba^{2+} events.**

References

[1] Nucl Instrum Methods Phys Res A 824:2–5 (2016).
[2] Nature 583, 48 (2020).
[3] Nat. Comm., 13, 7741 (2022).
[4] Sci Rep 9: 15097 (2019).
[5] ACS Sens, 6, 1, 192–202 (2021)
[6] JINST 18 P07044 (2023)
[7] *Papers in preparation.*