Stockholm University

Oskar Klein centre

PRINCETON UNIVERSITY

X-Disciplinary Hunt for Dark Matter: ML and Material Science Meet Astroparticle Physics

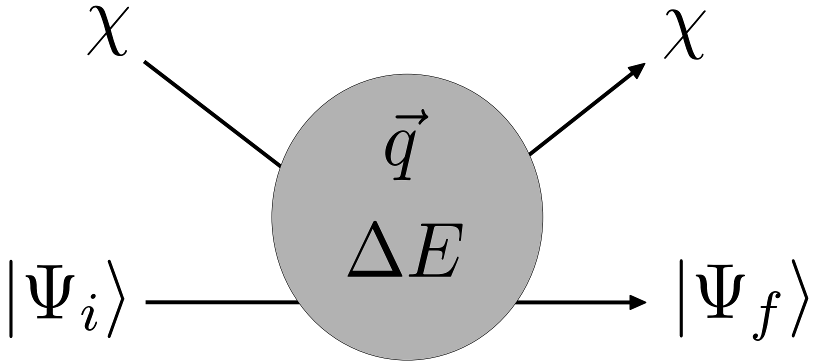
CARLOS BLANCO

NASA

SPACE TELESCOPE SCIENCE INSTITUTE

Direct Detection

$v \approx 10^{-3}$

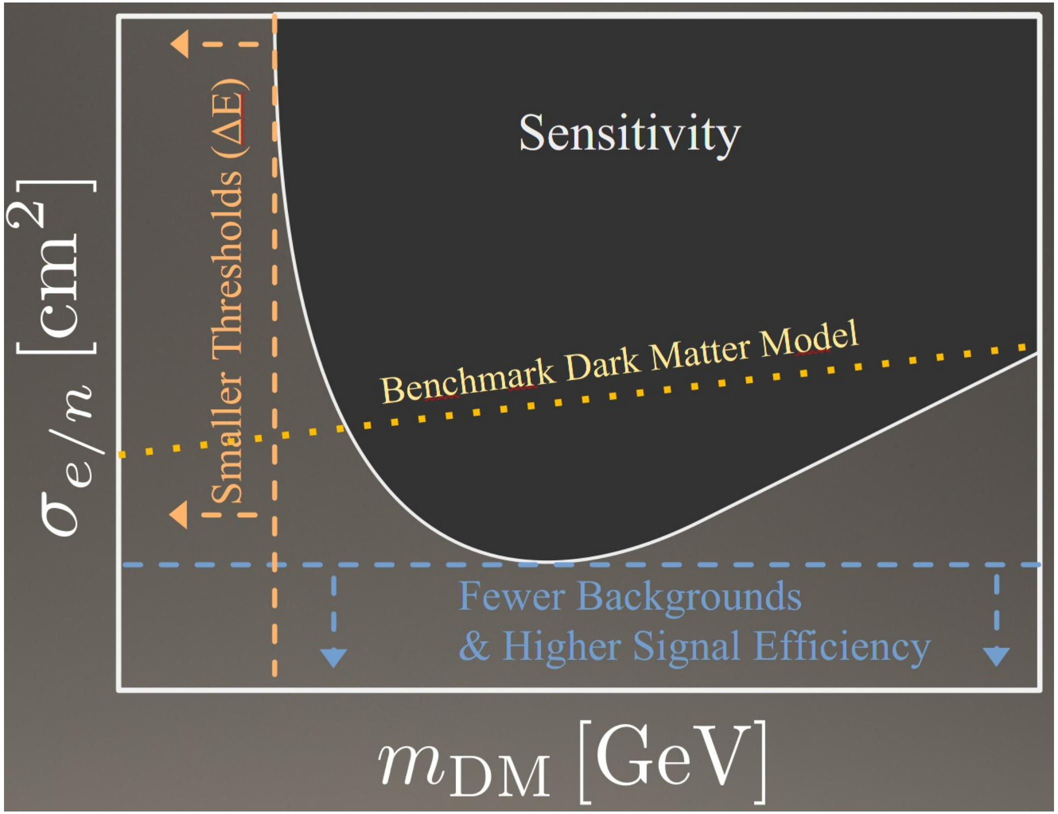


Energy Budget

$$\Delta E \sim v^2 m_\chi \approx \mathcal{O}(\mathrm{eV}) \left(\frac{\mathrm{m}_\chi}{1\,\mathrm{MeV}}\right)$$

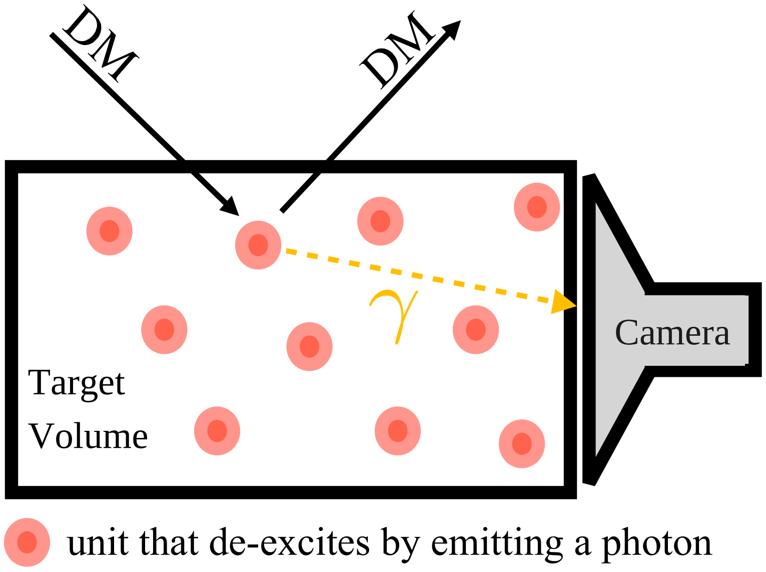
Momentum Budget

$$q \sim v m_\chi \approx \mathcal{O}(\mathrm{keV}) \left(\frac{\mathrm{m}_\chi}{1\,\mathrm{MeV}}\right)$$



Direct Detection: New Materials & Methods

Recoil-induced *fluorescense* (radiative deexcitation)

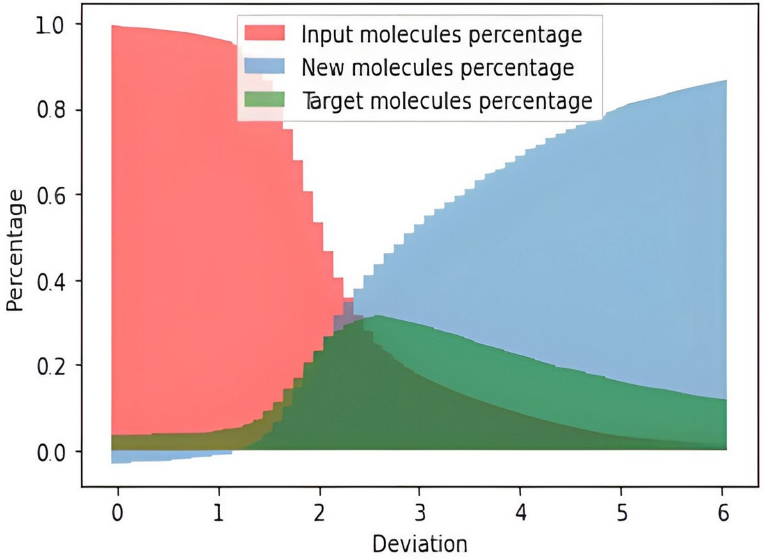


unit that de-excites by emitting a photon

Could be:

- Nanostructures (quantum dots)
- Molecules in ordered crystal
- Hybrid material (QDs in Molecular matrix)

ML to explore vast data of material space



Generative ML models will identify novel materials that maximize signals

Direct Detection: Interaction Rate

Rate *spectrum* (events in detector)

$$\Gamma \sim \int \frac{d^3\vec{q}}{q} \eta(v) |F_{\mathrm{DM}}(q)|^2 |f_{i\to f}(q)|^2$$

Mean inverse velocity (Astrophysics)

$$\eta(v)$$

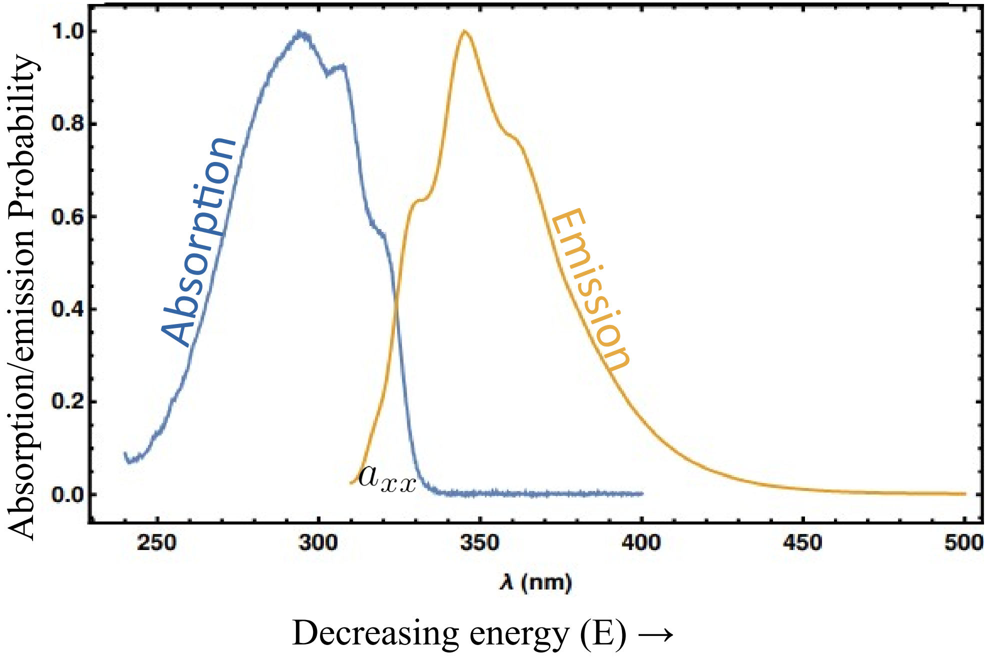
Transition form factor (Condensed matter / Chemistry)

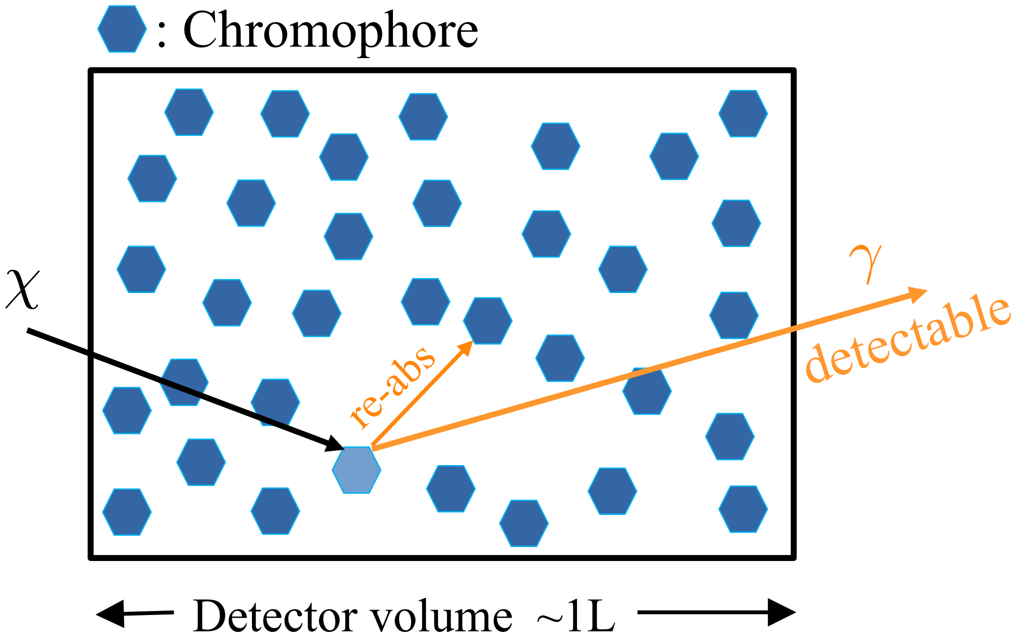
$$f_{i\to f}(q) = \langle \tilde{\Psi}_f(k+q) | \tilde{\Psi}_i(k) \rangle$$

Dark matter form factor (Particle physics)

$$F_{\mathrm{DM}}(q) \propto \begin{cases} 1 & \text{, Contact interaction} \\ \left(\frac{1}{q}\right)^2 & \text{, Long-range interaction} \end{cases}$$

Fluorescence with DM

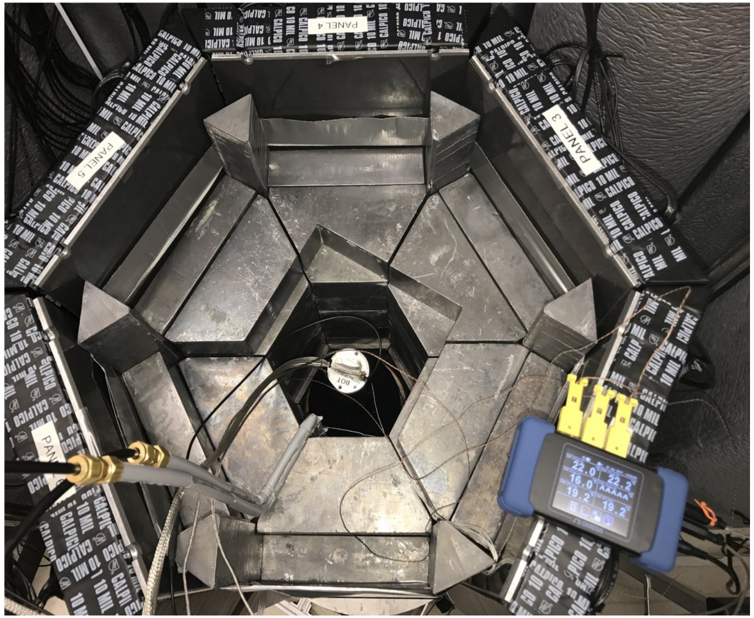


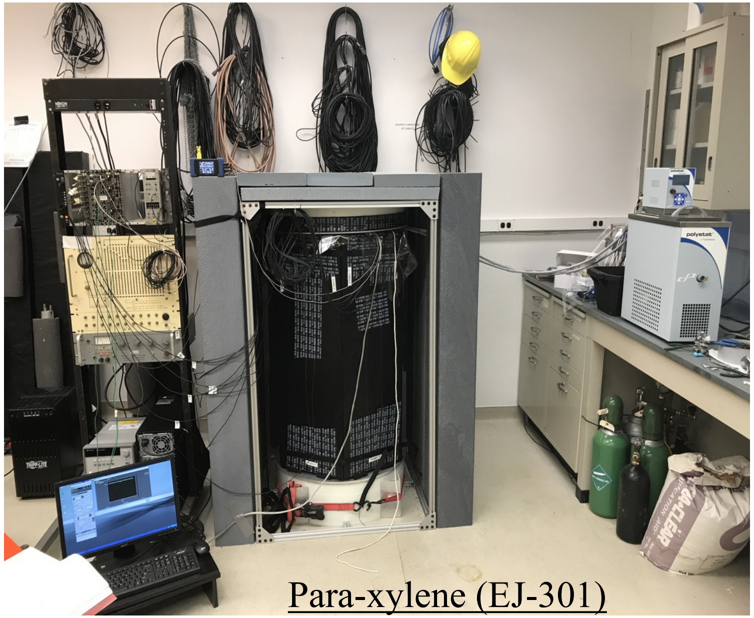


Probability for the photon to free stream

$\Phi_{\rm FB} \sim (1 - a_{xx})$ e.g. molecular crystals: $\Phi_{\rm FB} \approx 65\%$

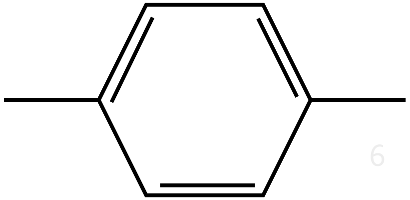
First Experimental Setup





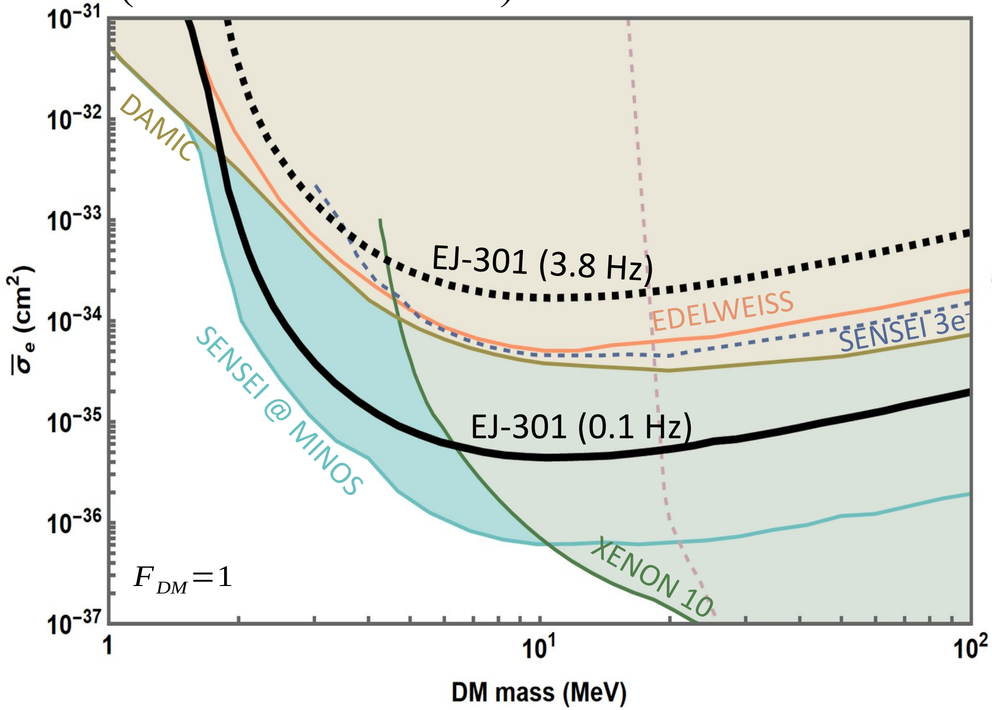
Para-xylene (EJ-301)

[**CB**, Collar, Kahn, Lillard: 1912.02822]

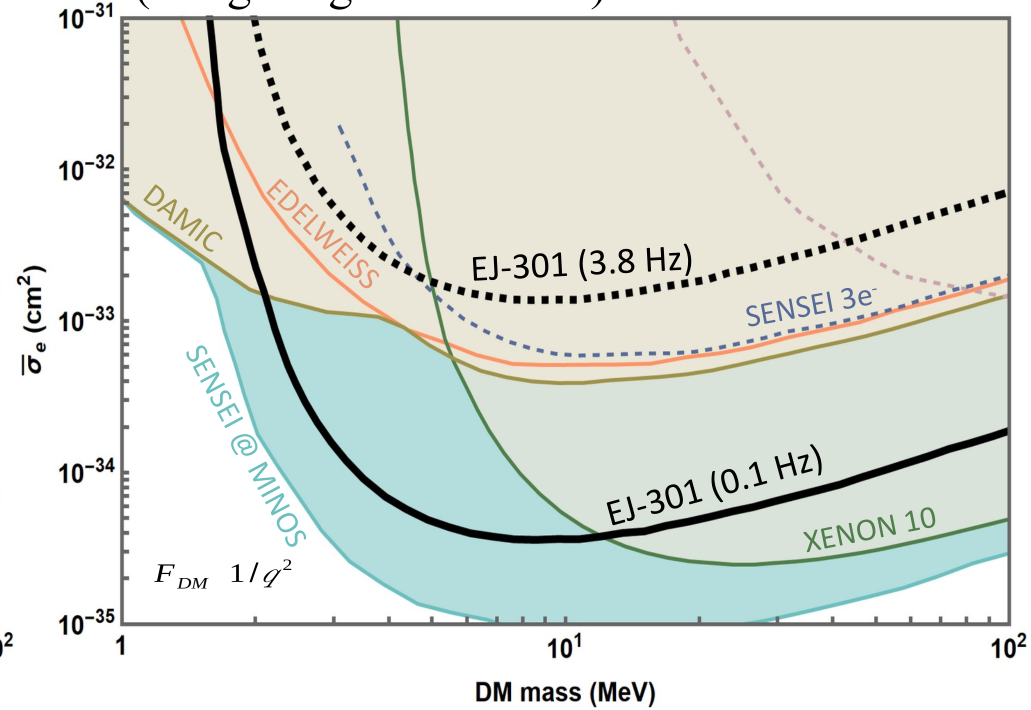


Results: EJ-301 (Xylene)

(Contact interaction)



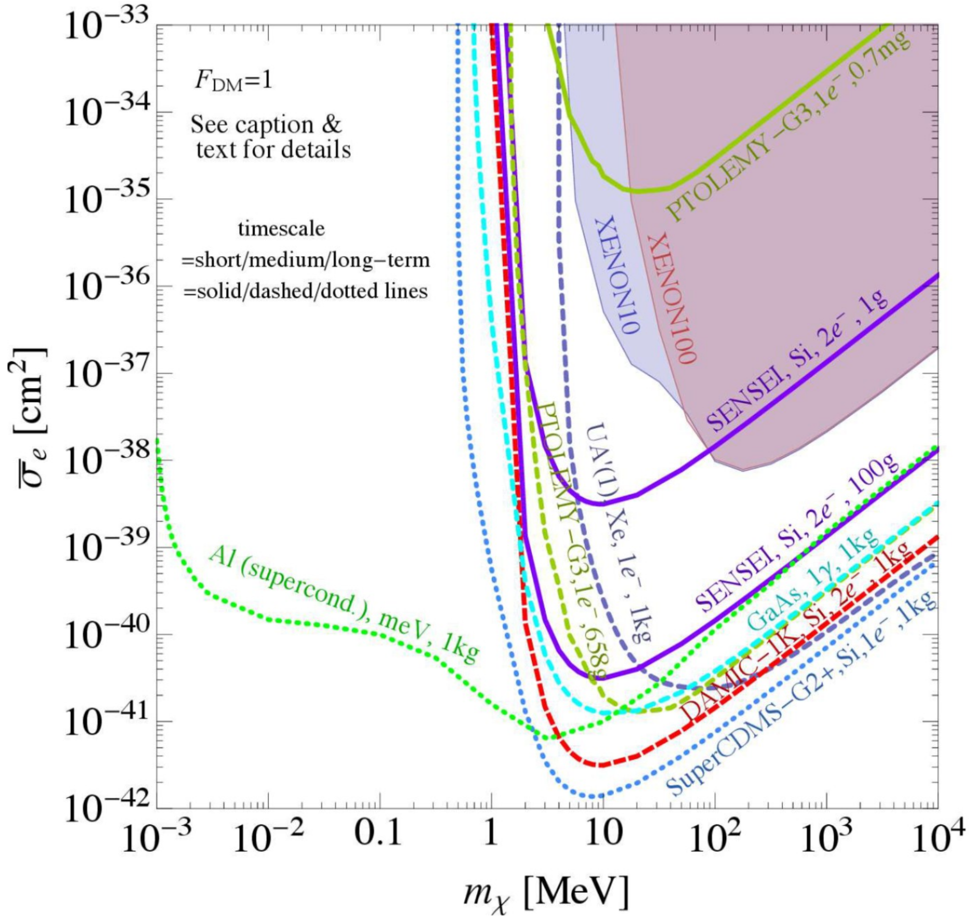
(Long-range interaction)



[**CB**, Collar, Kahn, Lillard: 1912.02822]

About 6 months from theory development to results.

The Field in Context



[US Cosmic Visions: Community Report: 1707.04591]

Many materials are proposed to probe the sub-GeV Space

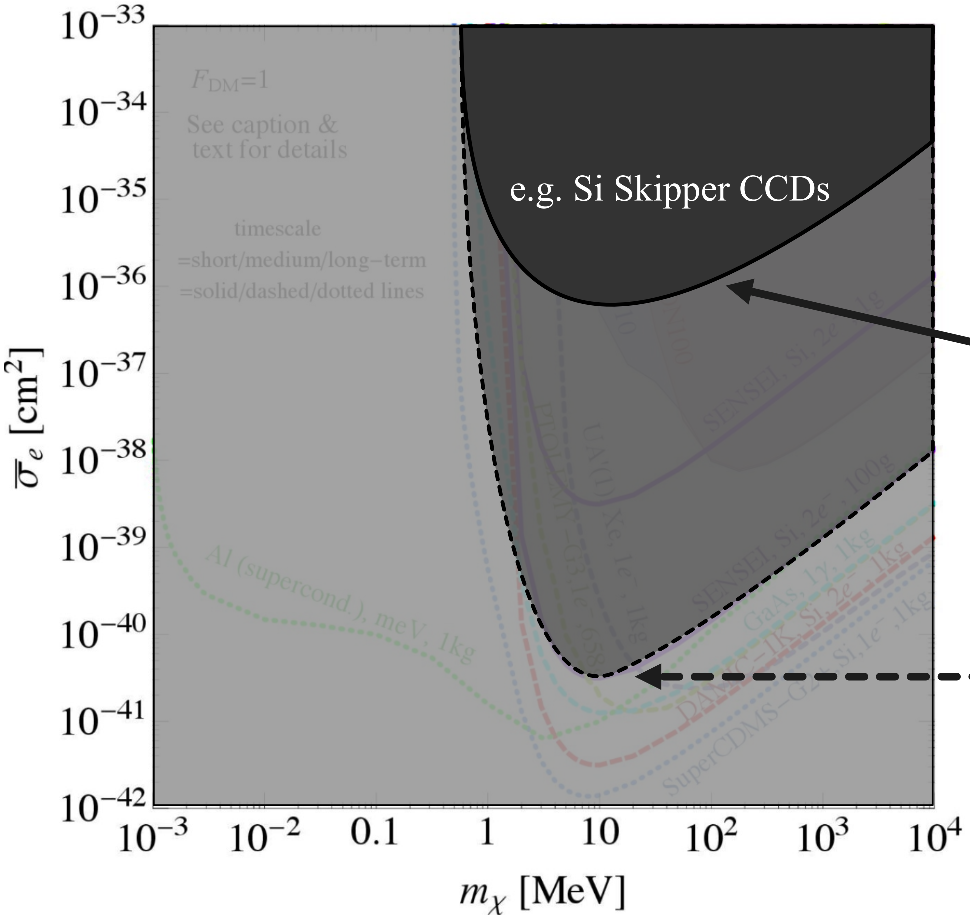
In 2017:

Short term (2 years)

Medium term (2-5 years)

Long term

Outlook and Potential Reach



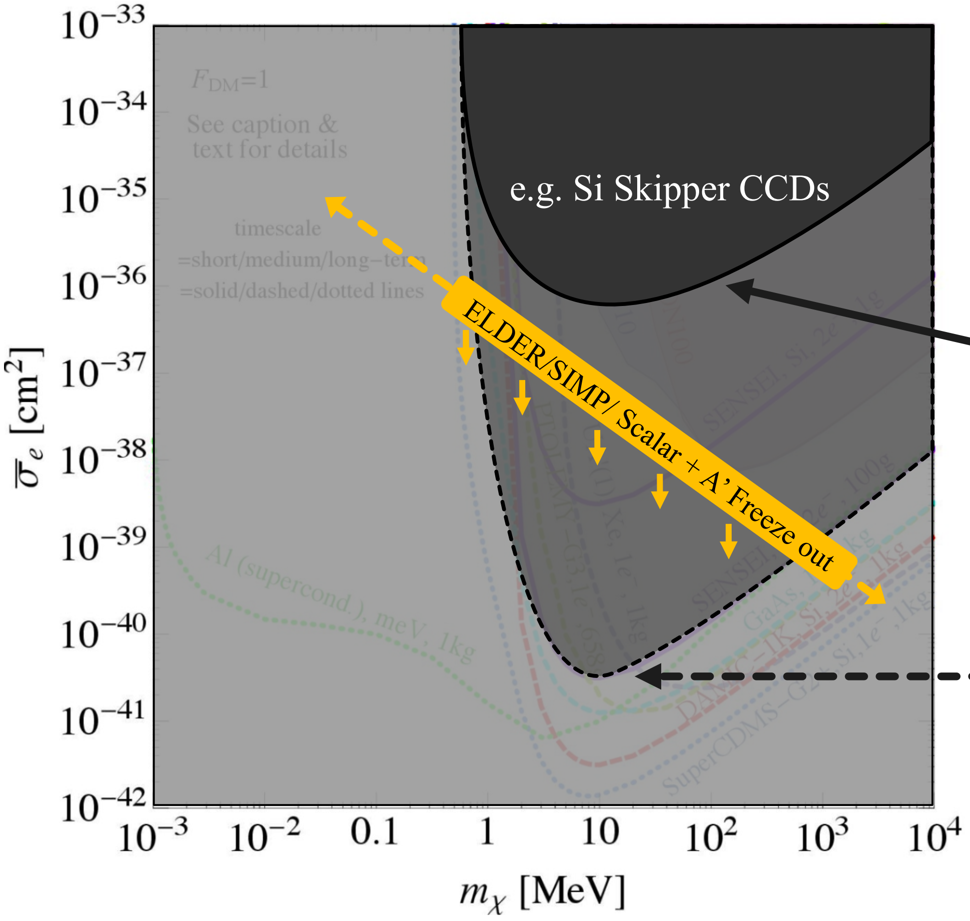
Present day:

Experimental results

Zero-background projection

[US Cosmic Visions: Community Report: 1707.04591]

Outlook and Potential Reach



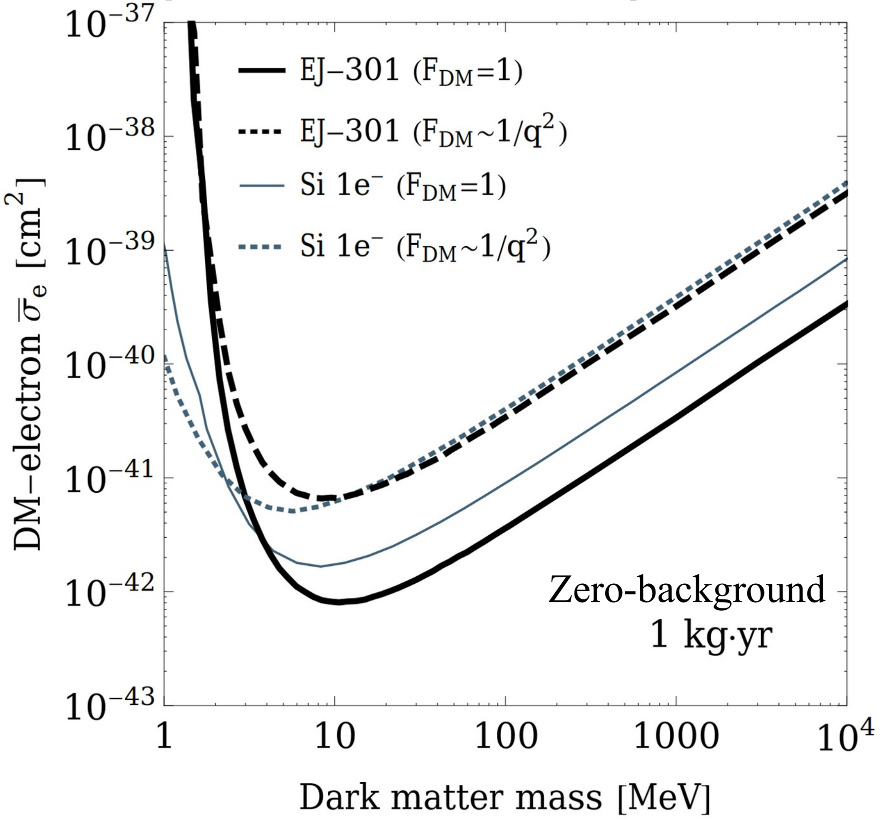
Present day:

Experimental results

Zero-background projection

Outlook and Potential Reach

[**CB**, Collar, Kahn, Lillard: 1912.02822]



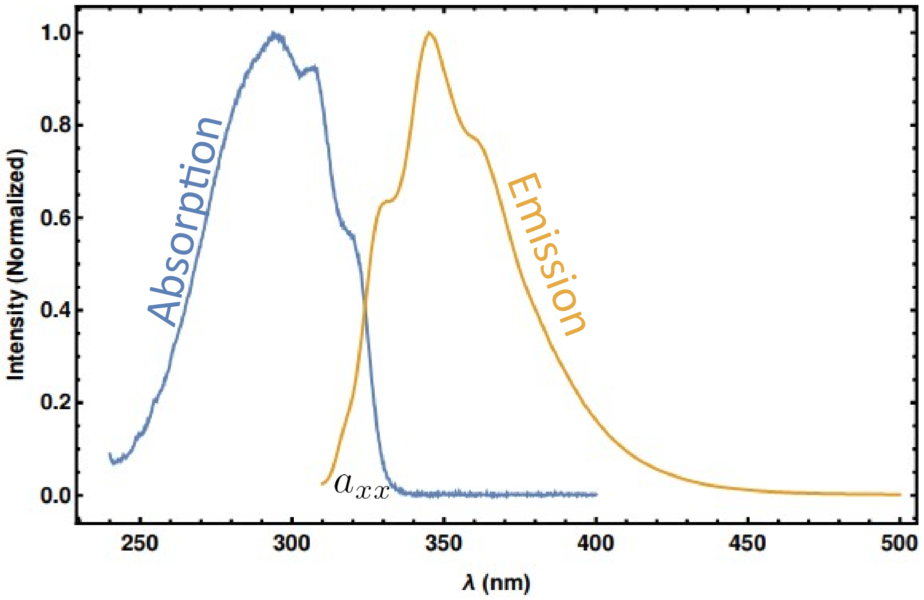
The obstacle

Backgrounds

6 orders of magnitude of potential reach awaiting

Pound (kg) for Pound (kg) molecules produce about as much signal as e.g. Si.

Fluorescence with DM



Option 1

Reduce background in the excitation.

Molecular crystals

Anisotropic excitation → Time-varying DM signal

Next Step

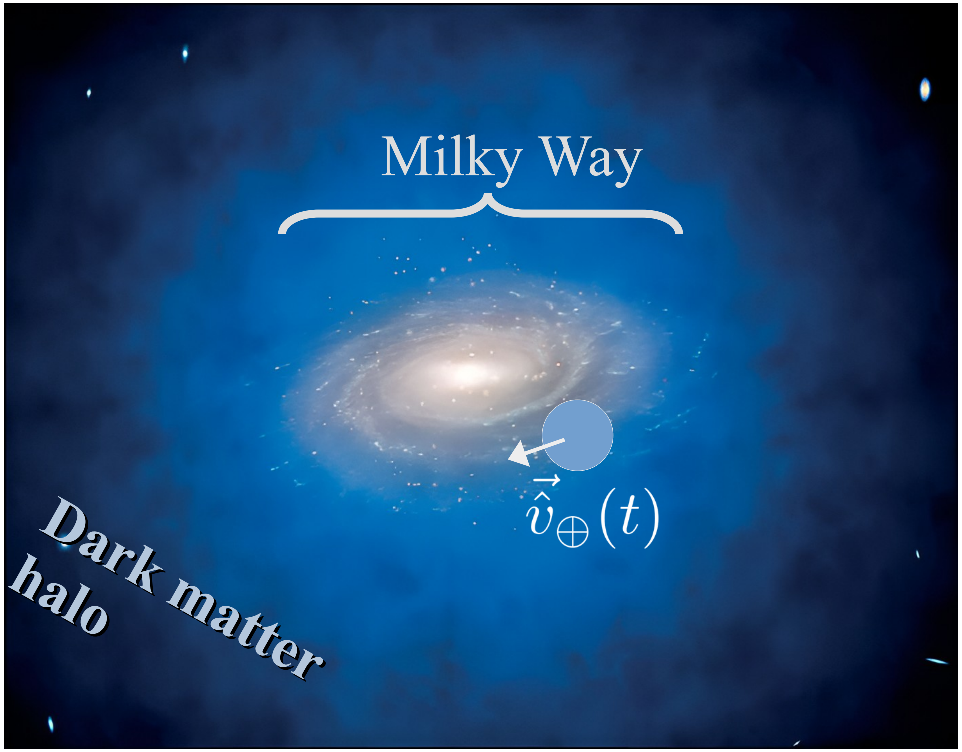
Option 2

Reduce background in the emission.

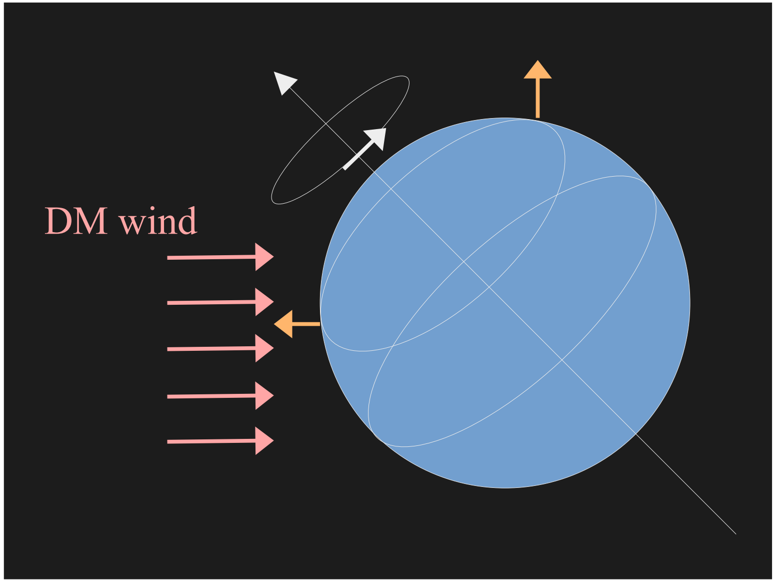
Quantum dots

Multiple excitons → Time-coincident DM signal

Directional Detection

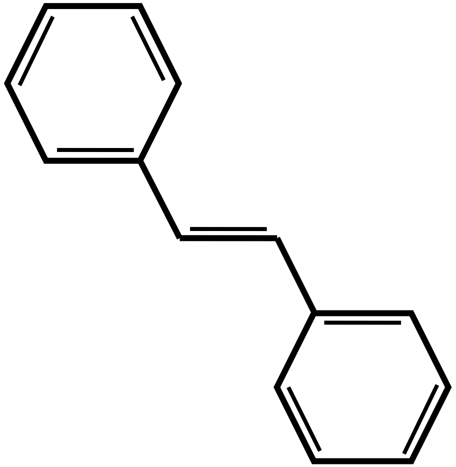


Effective dark matter "wind" from relative motion

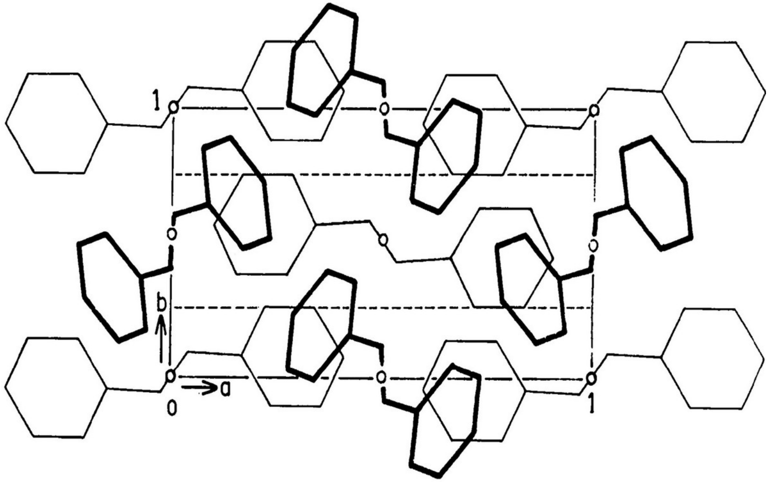


Change in relative orientation between detector and dark matter wind leads to ***daily*** modulation

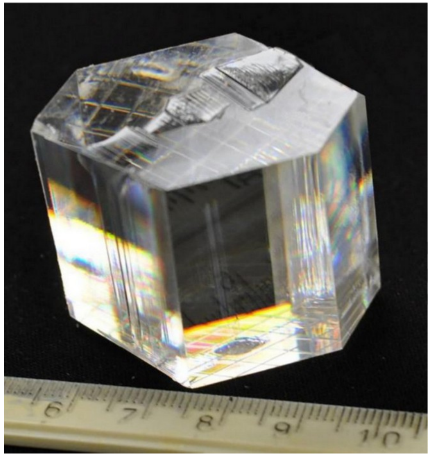
Trans-Stilbene



Delocalized and planar network of double bonds



Molecular planes oriented in crystal lattice

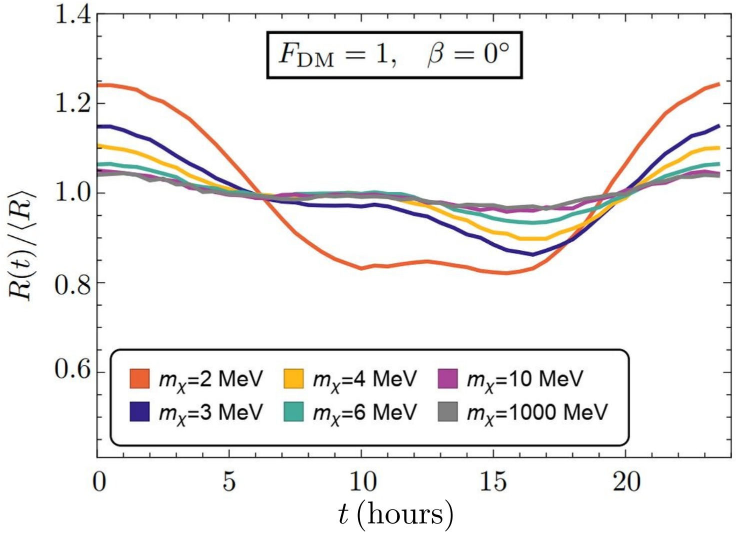


Carman, et.al. '18 (J. of Crystal Growth)

Large optical-quality crystals

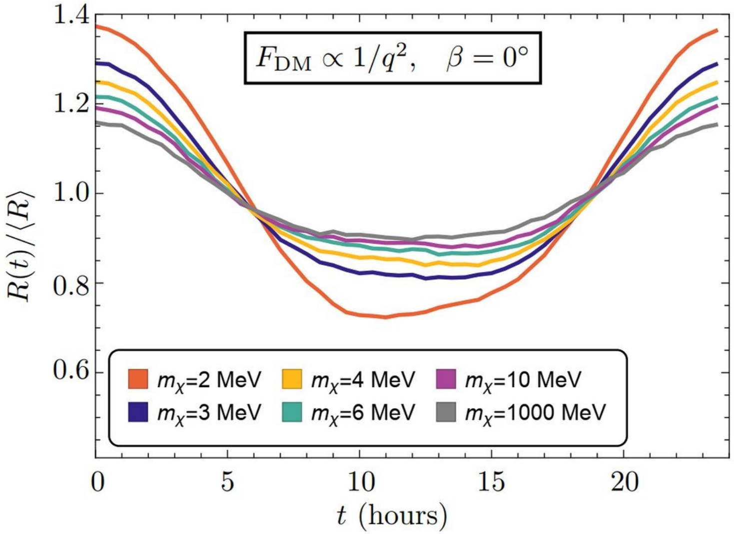
Daily Modulation

(Contact interaction)



[**CB**, Kahn, Lillard, McDermott: 2103.08601]

(Long-range interaction)

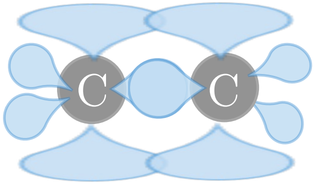


Varies up to 70%

Verifiable signal!

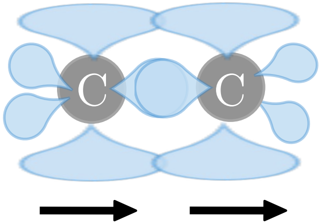
Modulation amplitude remains as high as 10% even at the highest masses due to the fundamental anisotropy of the molecular form factor.

The Molecular Migdal Effect(s)



Center of mass recoil (CMR)

Cause by center of mass motion



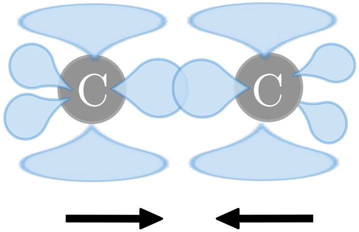
Analogous to atomic Migdal effect

$$P_{CMR} \sim \frac{m_e}{M_{mol}}$$

Moving whole molecule → BIG penalty

Non-adiabatic coupling (NAC)

Caused by relative motion

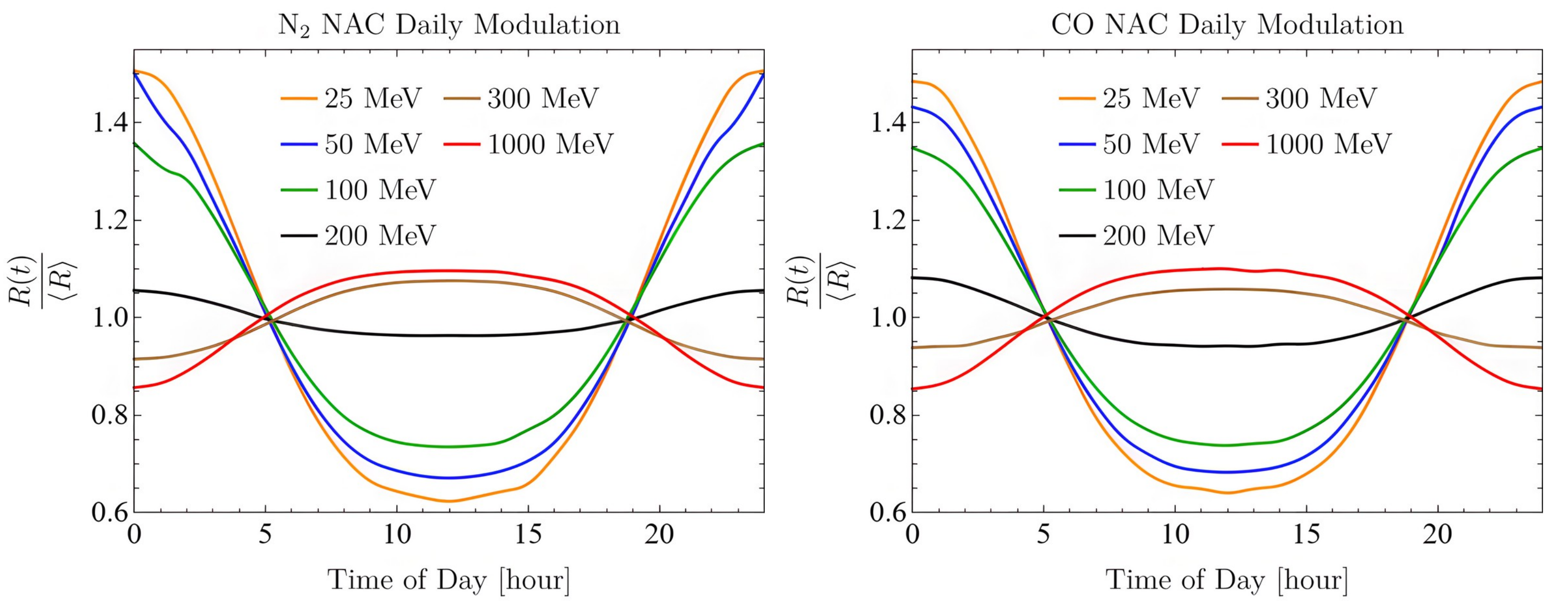


Effect beyond Born-Oppenheimer

$$P_{NAC} \sim \frac{m_e}{M_N}$$

Crumpling molecule → small Penalty

Directional Molecular Migdal Effect



[**CB**, Harris*, Kahn, Lillard, Perez-Rios: 2208.09002]

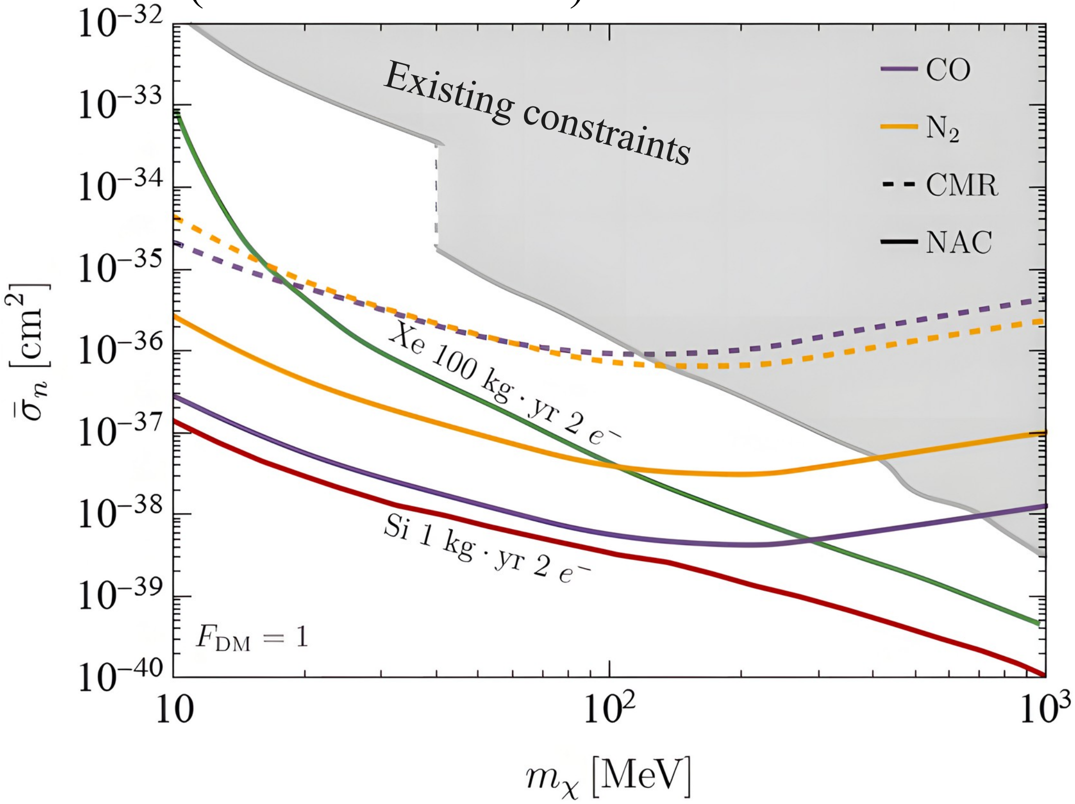
Varies up to 80%

Mass dependent phase

Molecular alignment → Directional electronic excitation → Directional molecular Migdal effect(s)

Molecular Migdal Effect(s)

(Contact interaction)



[**CB**, Harris*, Kahn, Lillard, Perez-Rios: 2208.09002]

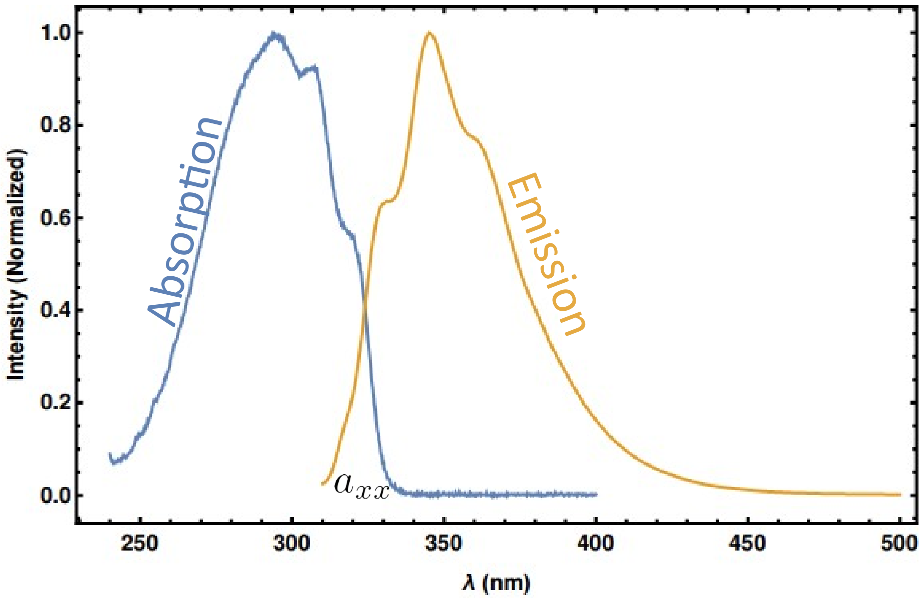
Si rate is calculated using the *CMR*-equivalent Migdal effect.
Is there an *NAC*-equivalent in Si?

enter of mass recoil
Subdominant at all masses.

Non-adiabatic coupling
Favorable kinematic factor.

Simplest molecular models already competitive.

Fluorescence with DM



Next Step

Option 1

Reduce background in the excitation.

Molecular crystals

Anisotropic excitation → Time-varying DM signal

Option 2

Reduce background in the emission.

Quantum dots

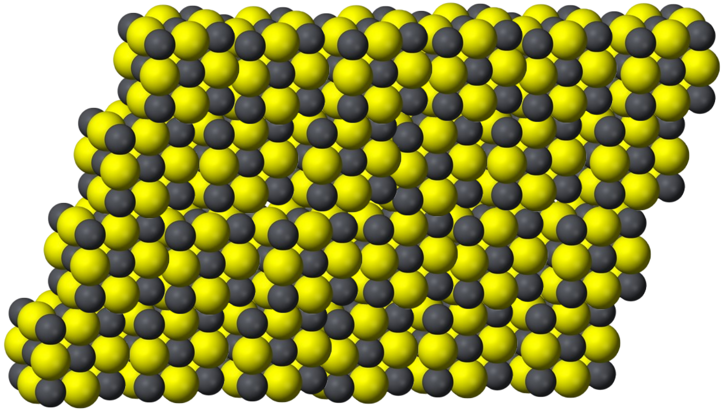
Multiple excitons → Time-coincident DM signal

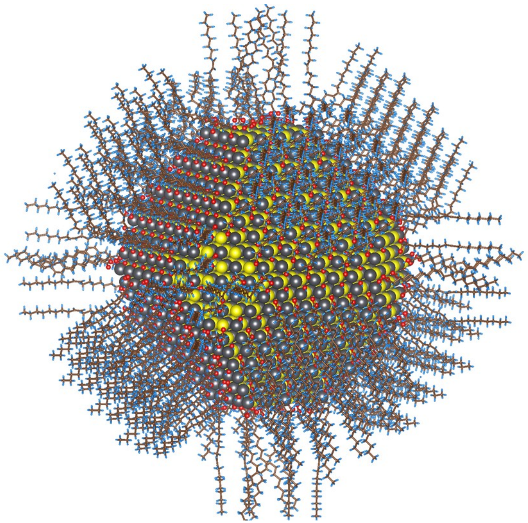
Nanocrystals: Quantum Dots

Quantum confinement affects long-wavelength physics

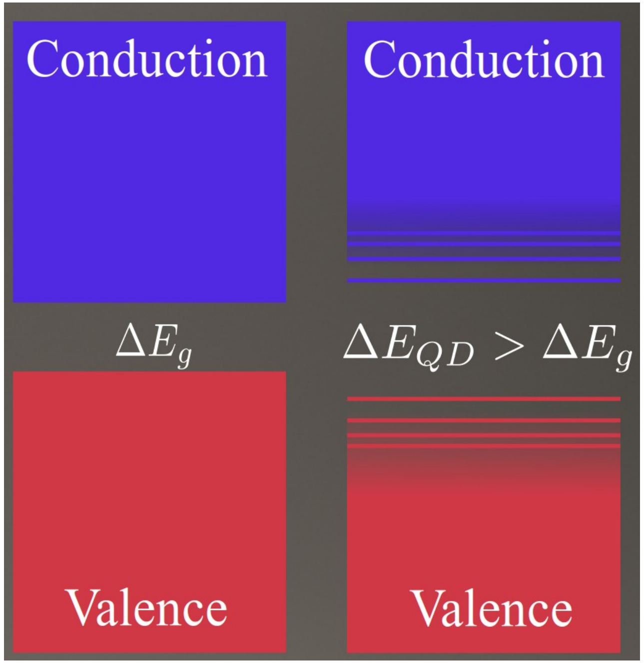
Quantum confinement

Example: PbS





Zherebetskyy et al., Science 344, 1380 (2014)



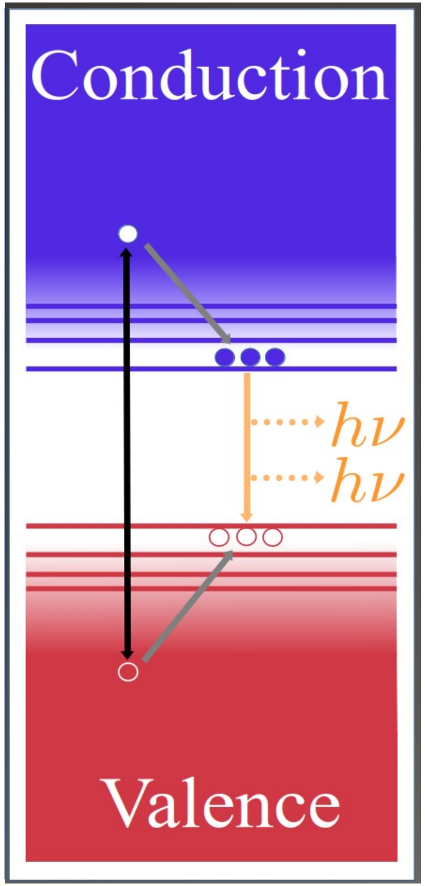
$R \to \infty$

$R \sim \mathcal{O}(\text{few nm})$

$|\psi_i\rangle \sim u_{\text{Bloch}}(r)e^{ik\cdot r}$

$|\psi_i\rangle \sim u_{\text{Bloch}}(r)\psi_{\text{bound}}(r)$

Quantum Dots: Coincident Signal



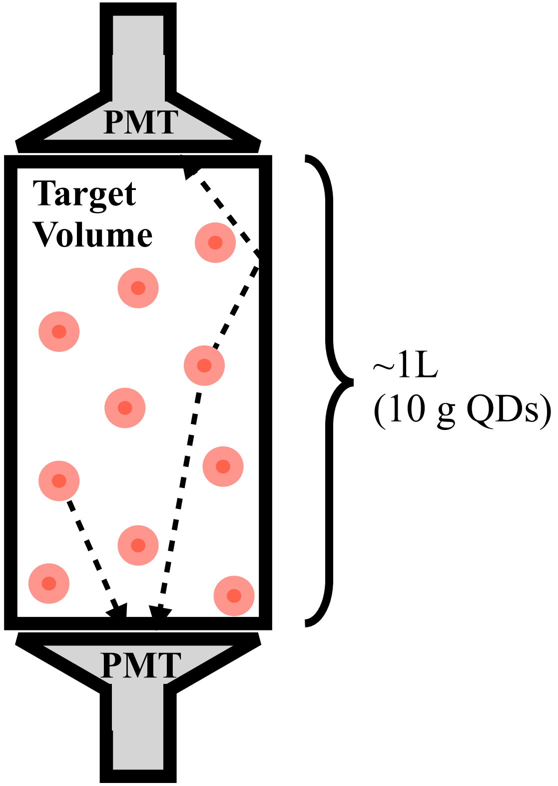
Absorption → Very *energetic* exciton

Multi-exciton generation → several excitons

If energy is greater than twice the band gap

Radiative recombination → coincident photons

Band-edge excitons produce light



Deployment: DarkDot & QUADRA

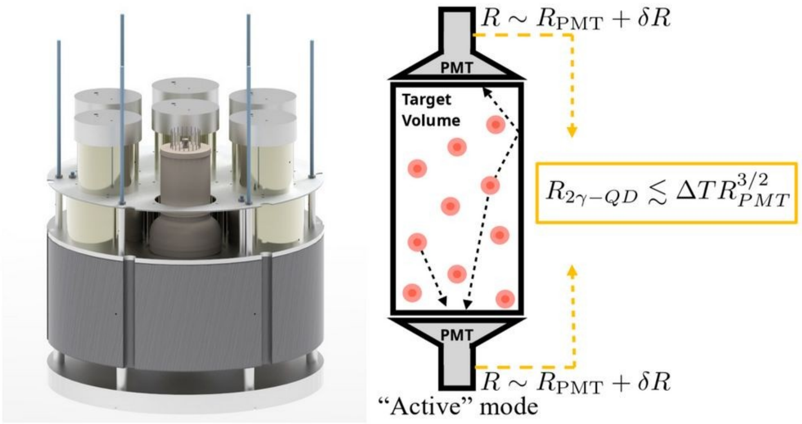
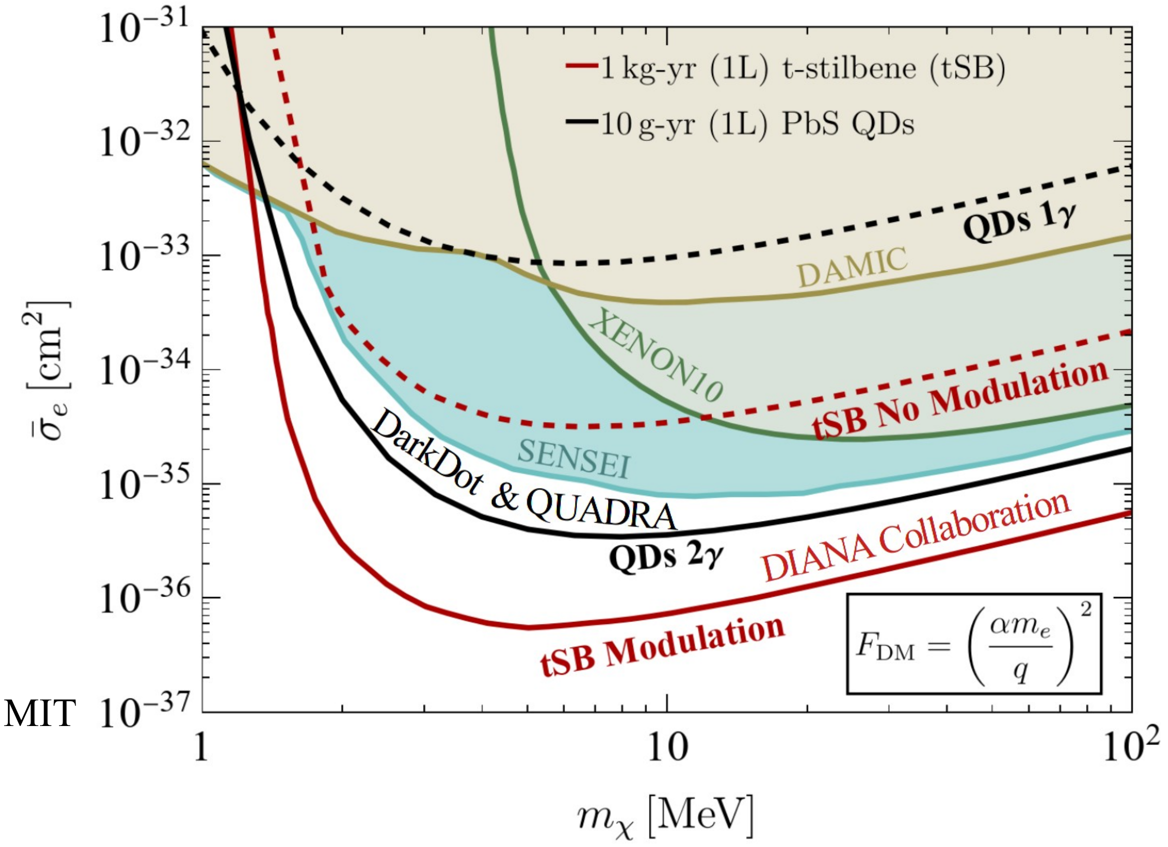


Figure 2: (Left:) Inner structure of the current SUXESs facility. (Right:) A diagram of a single module for the proposed detector.



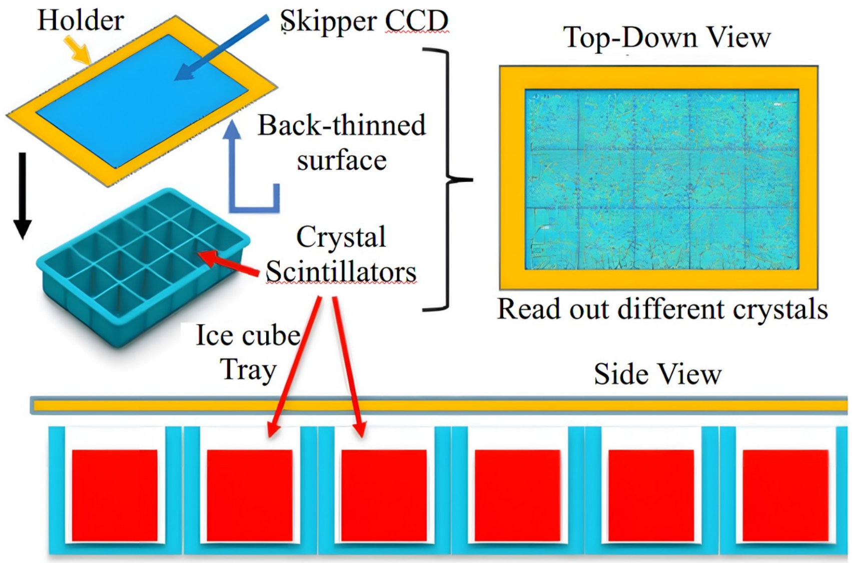
Experimental Collaborations

DarkDot (SNSPDs): MIT (Host), Stockholm U.

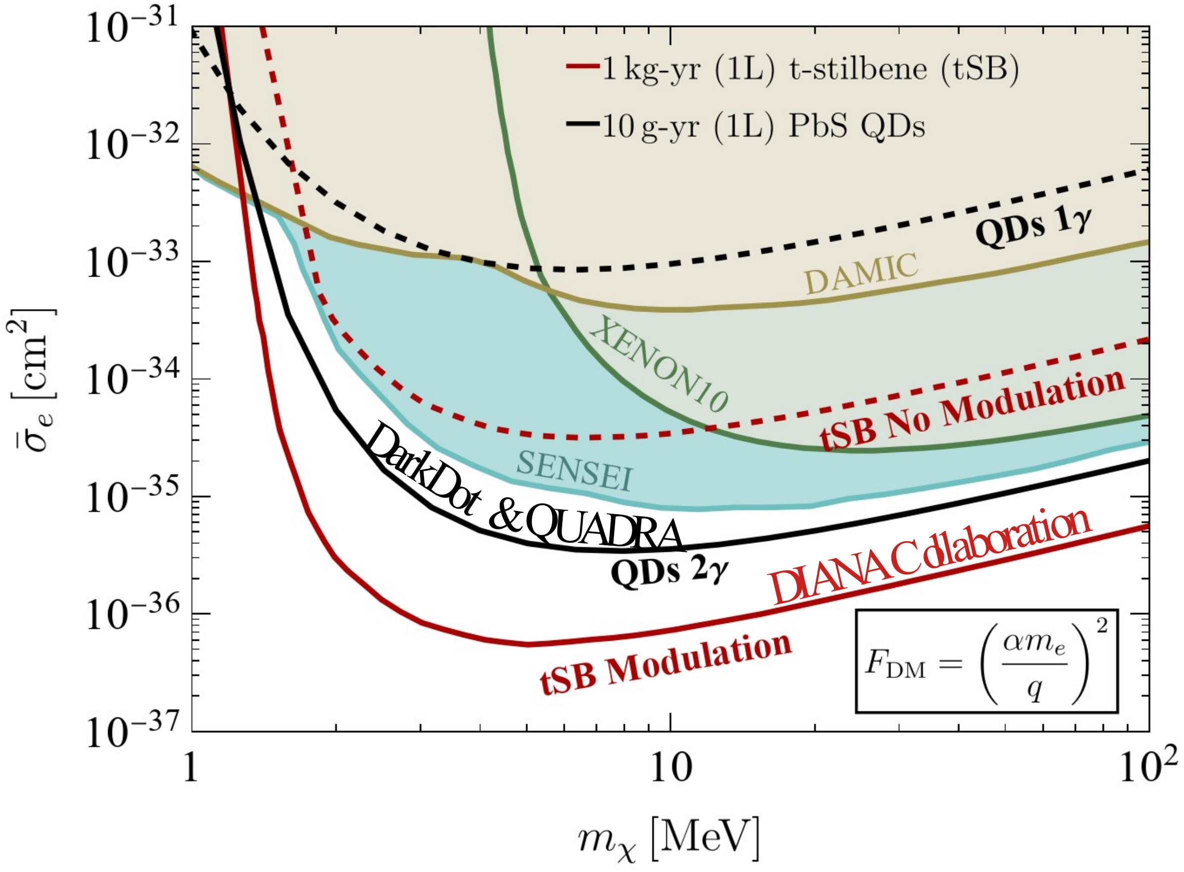
QUADRA (Abalone PMTs): Stockholm U. (Host), MIT

Deployment: DIANA*

Daily Modulation in an Intrinsically ANisotropic Array

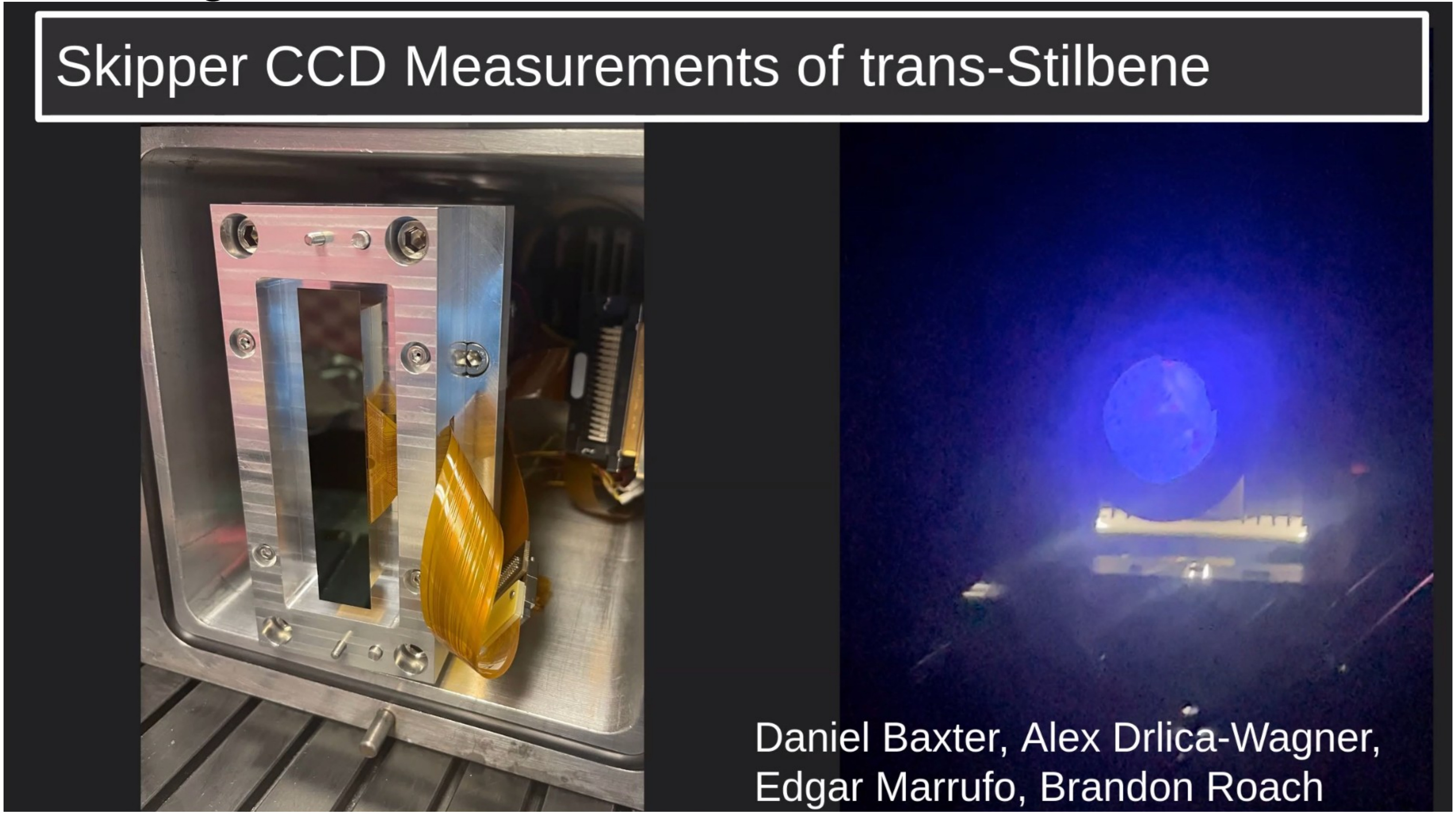


Collaboration: FermiLab, MIT, UIUC, U. Oregon



Deployment: t-stilbene

Detecting fluorescence with Si



Deployment: t-stilbene

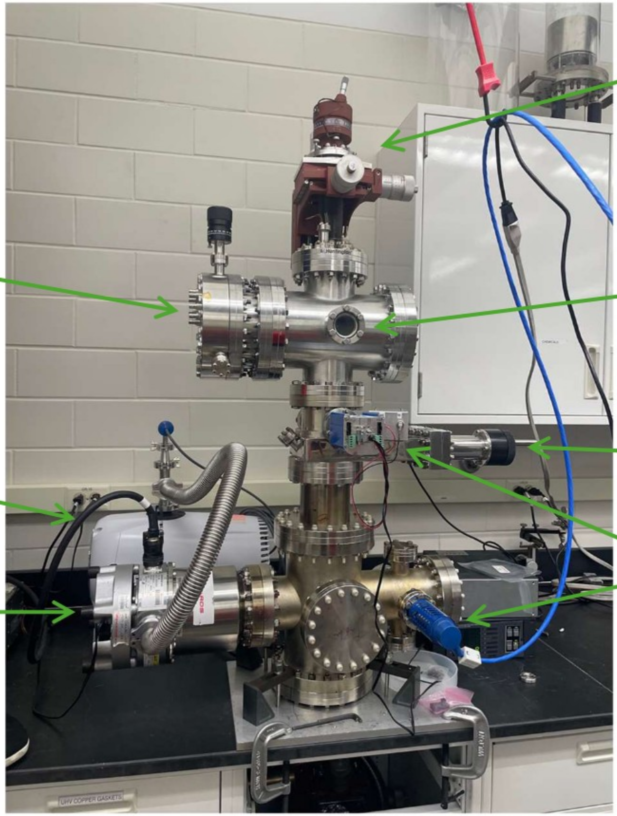
Calibration of anisotropy

Angle-dependent stilbene fluorescence gizmo (ADSFG)

Electron gun (10-250 eV) + phosphor screen for LEED

Scroll pump

Turbo, 500 l/s for "overpumping"



Sample manipulator (x,y,z,θ) for rotating stilbene crystal

Viewport for PMT (not shown but working)

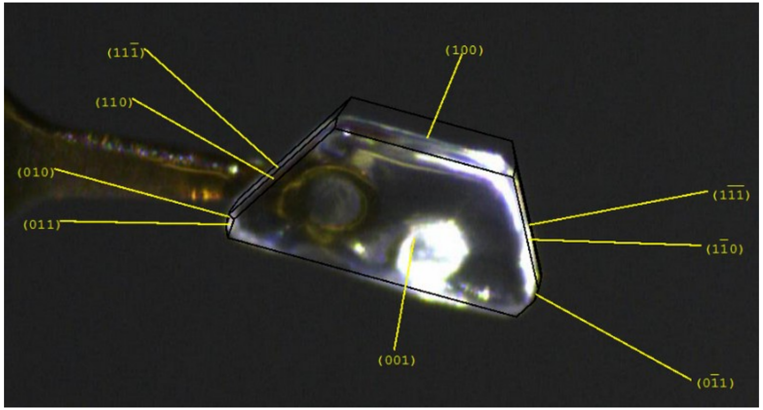
Gate valve

Ion Gauges

Abbamonte Group (UIUC)

Deployment: t-stilbene

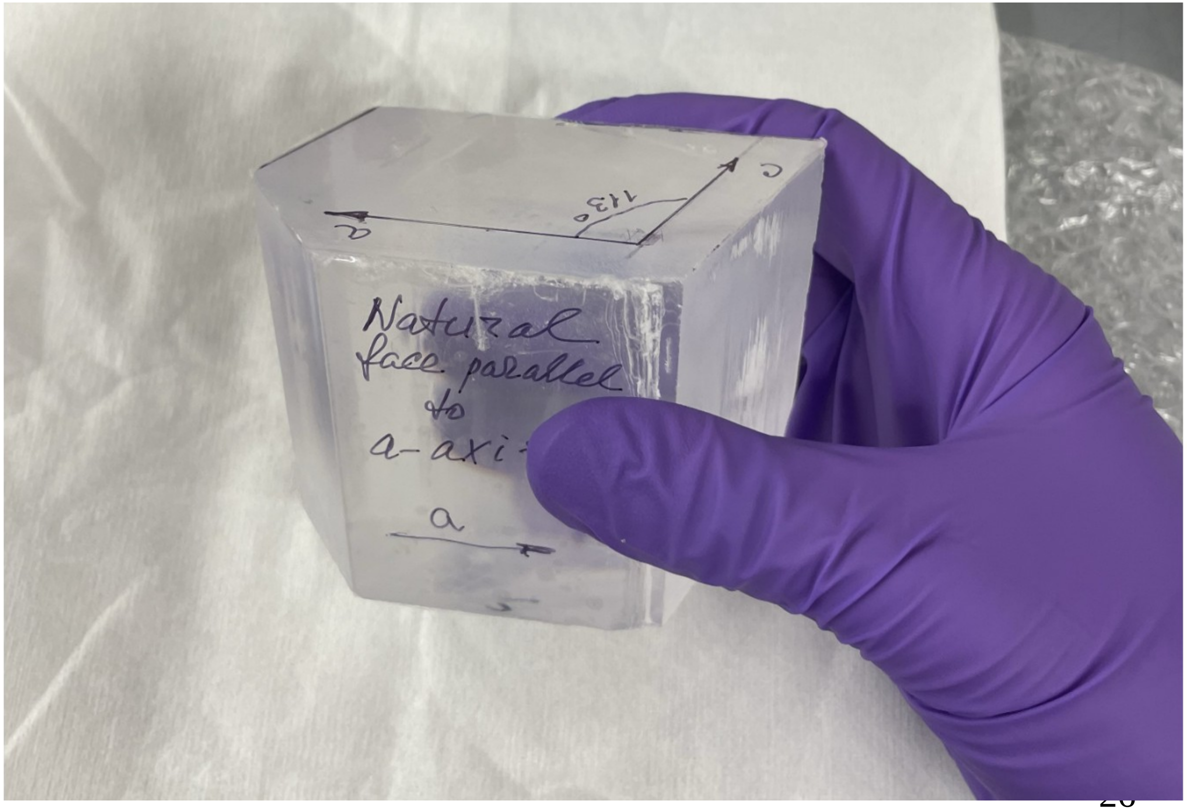
Calibrate at mg-scale



Credit: Dane Johnson
Freedman Group (MIT)

Natalia Zaitseva (LLNL)

Scale to kg-scale



Finding Optimal Targets

Problem: Chemical space is unreasonably large

How many molecules possible with
C, O, N, F, H?

< 9 atoms: 100s of Thousands (DFT Computable)

< 30 atoms: 100s of Billions (Intractable)

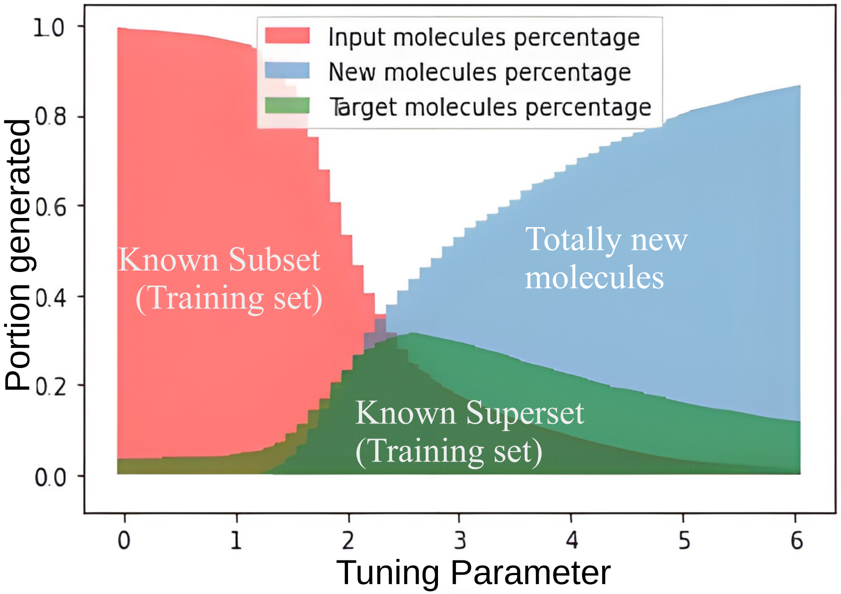
...toluene has 15, xylene has 18, t-stilbene has 26

Method

1. Look for known favorable properties - *cheminformatics*
2. Extra(intra)polate ont

ML for DM Direct Detection

Property prediction Molecular Generation



[**CB**, Cook*, Smirnov: 2411.xxxxx]

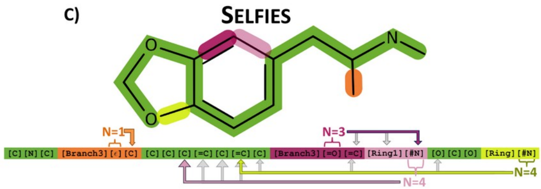
Using exhaustive database (< 9 atoms)
Characterize neural nets
→ Possible to learn from small subsample

Next: Large but sparse dataset up to 10s of atoms

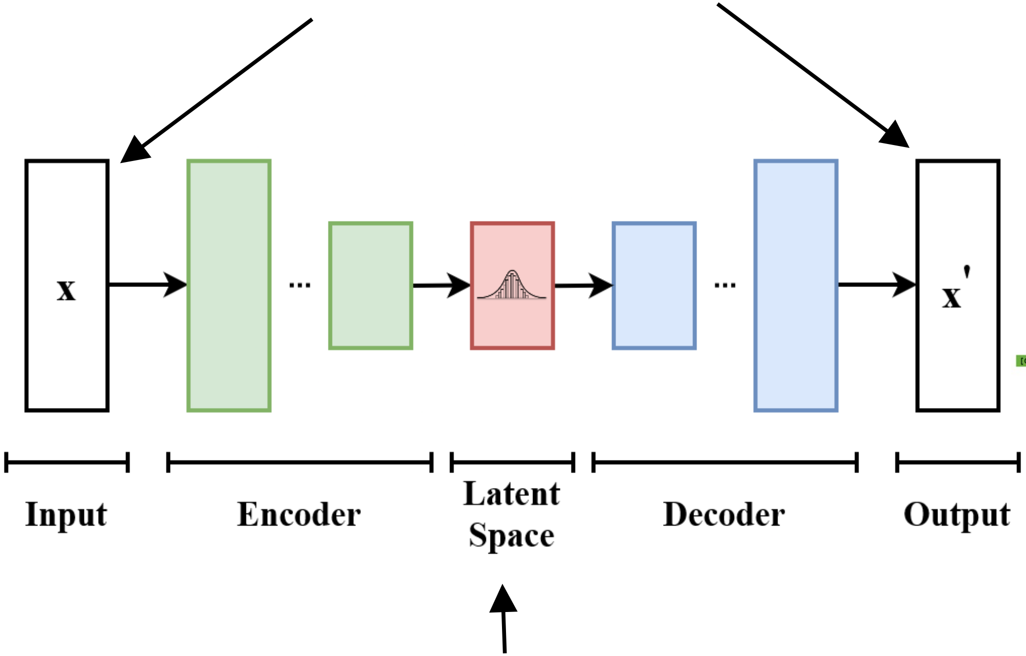
ML for DM Direct Detection

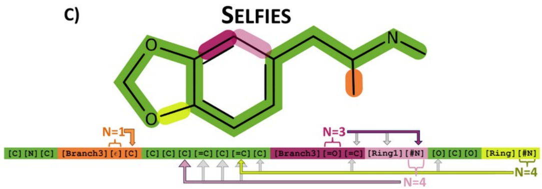
Molecular Space: Variational Autoencoders

Discrete and sparse data space



[Krenn et al : 1905.13741]



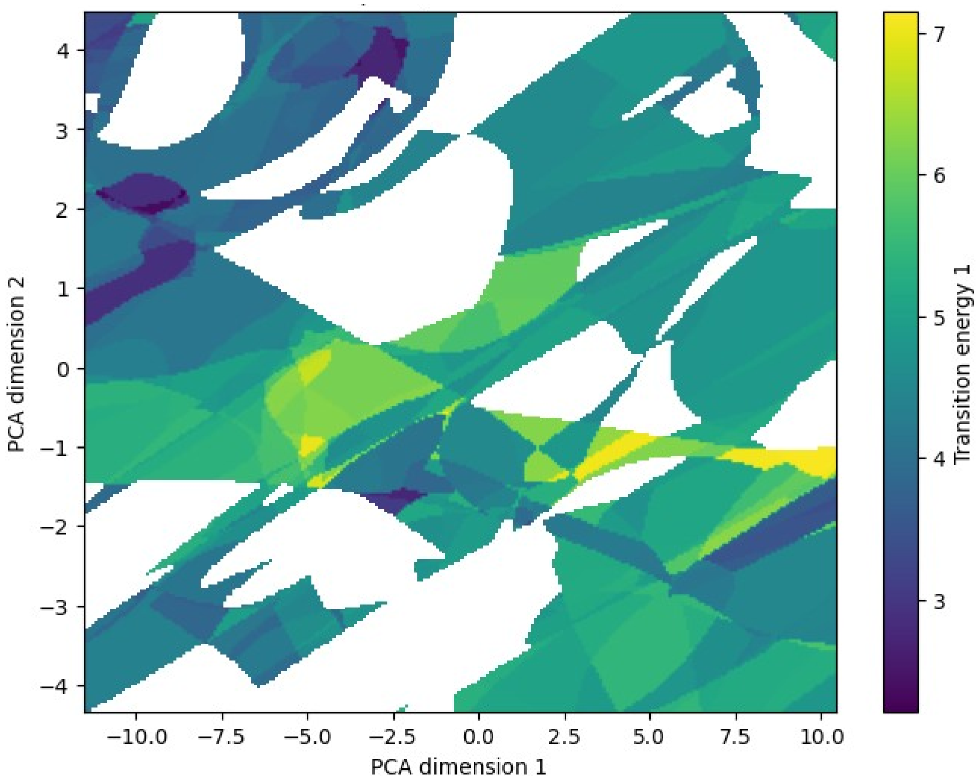


Continuous latent space

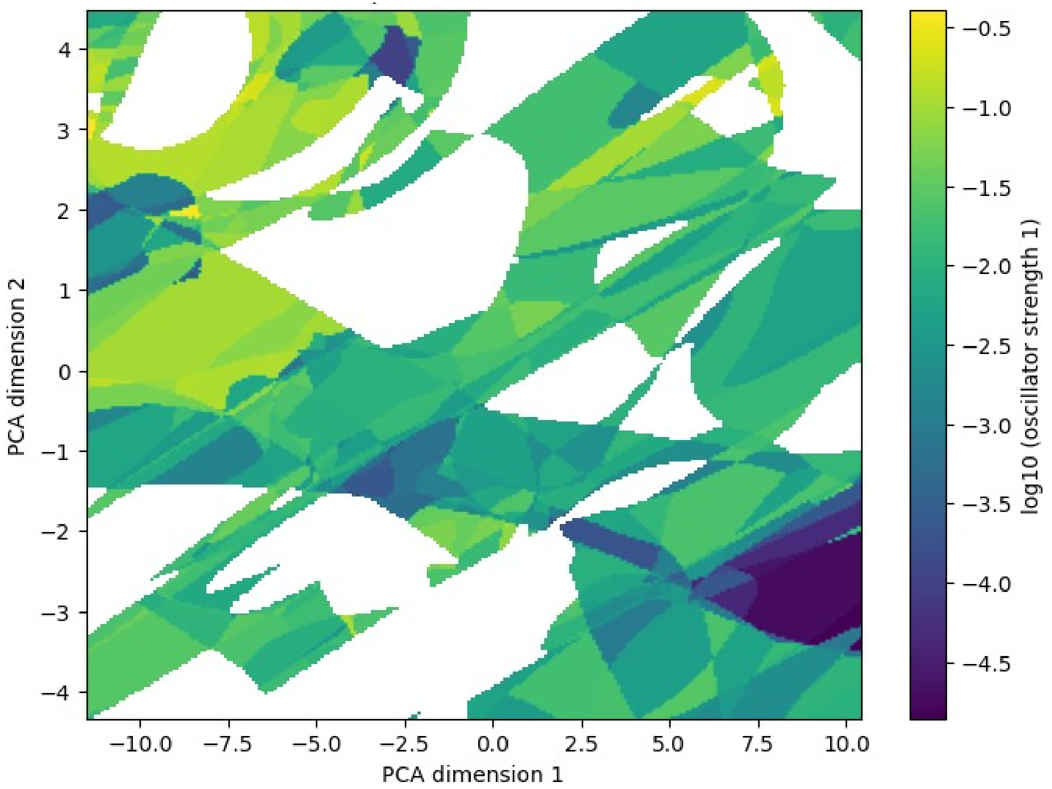
ML for DM Direct Detection

Property prediction: Molecular latent space

ΔE



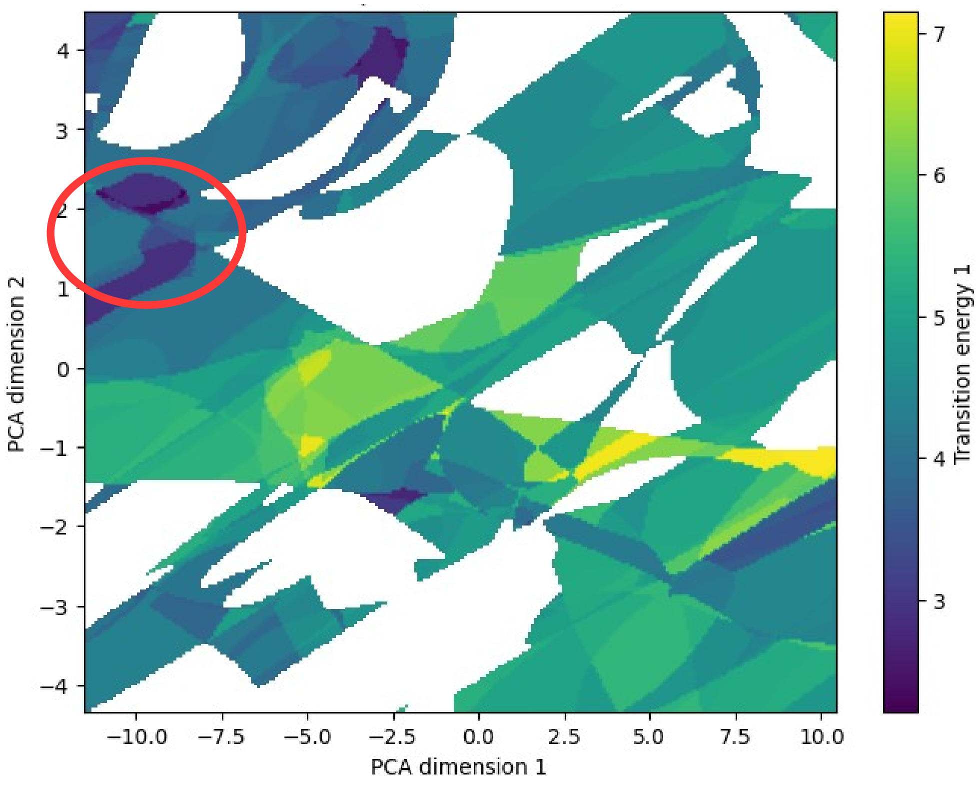
$\langle r_{01} \rangle \approx |f_{0,1}|/q$



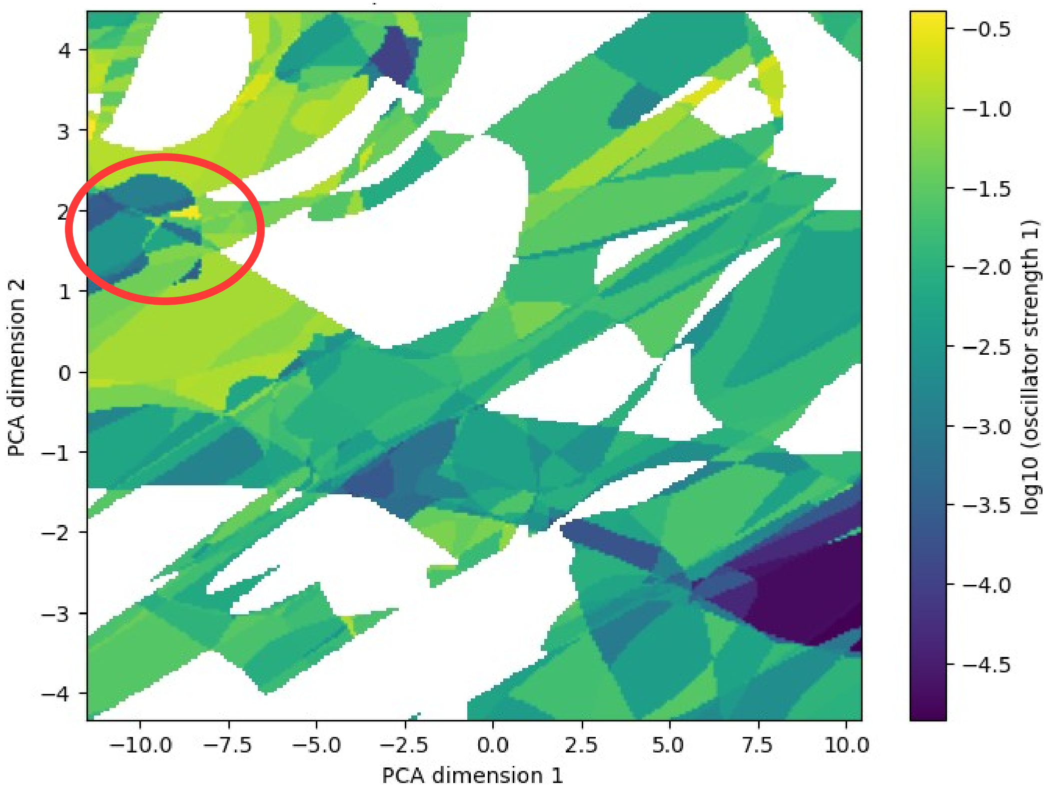
ML for DM Direct Detection

Property prediction: Molecular latent space

ΔE

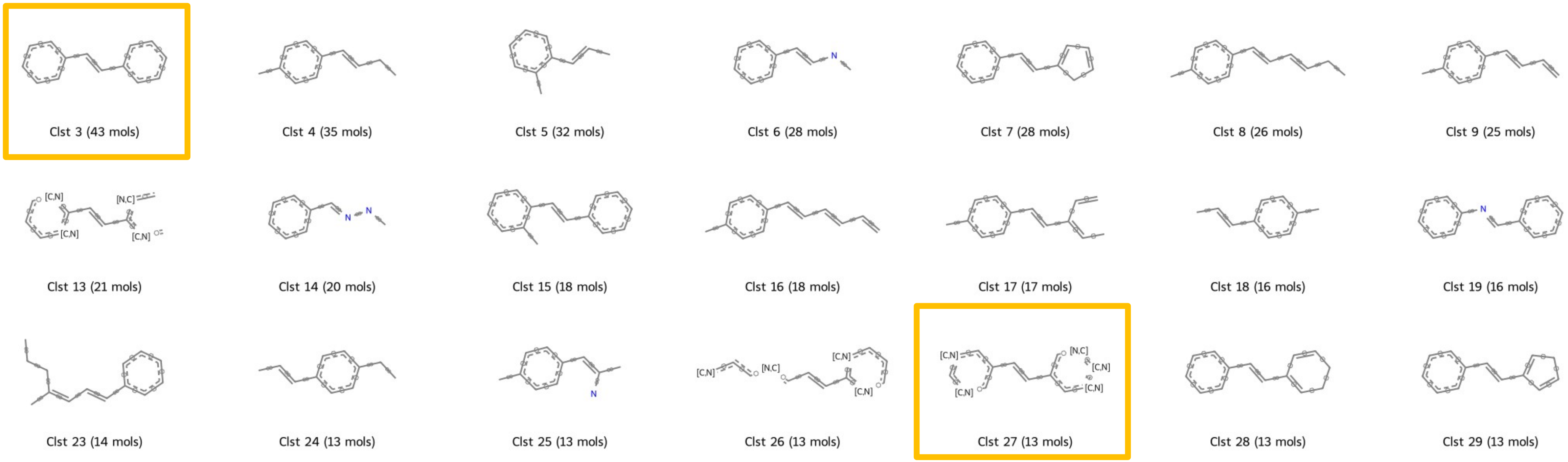


$\langle r_{01} \rangle \approx |f_{0,1}|/q$



ML Proposed Molecules

Property prediction Molecular Generation



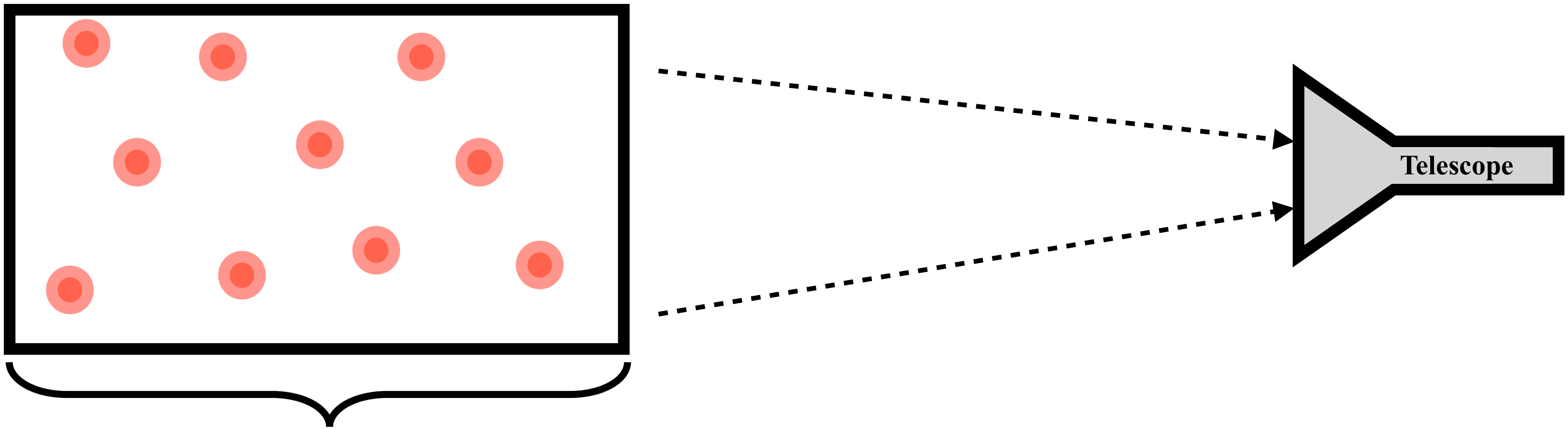
Molecular generation

→ Generate candidate molecule *shortlist:* Min($\Delta E \sim 2$eV), Max($\langle \vec{r} \rangle$), filter for synthetic feasibility.

→ Cluster by molecular similarity

→ Extract largest common substructure

Beyond direct detection



Astrophysical volume of molecules

Same theoretical techniques → Predict rates in *astrophysical* objects

Dark Matter can be captured inside celestial objects.

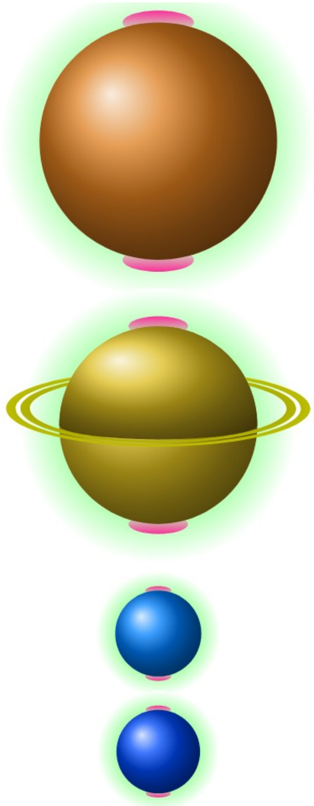
Assuming equilibrium is reached:

$$\Gamma_{\rm ann} = f_{\rm cap} \times \pi R^2 \rho_\chi v_\chi \sqrt{\frac{8}{3\pi}} \left(1 + \frac{3}{2}\frac{v_{\rm esc}^2}{v_\chi^2}\right)$$

Geometric scaling

Enhancement due to gravity

$$P_{\rm ion}^{\rm DM} = \frac{\Gamma_{\rm ann} \times f_{\rm iono}}{4\pi R^2}$$



Equilibrium Radial Distribution

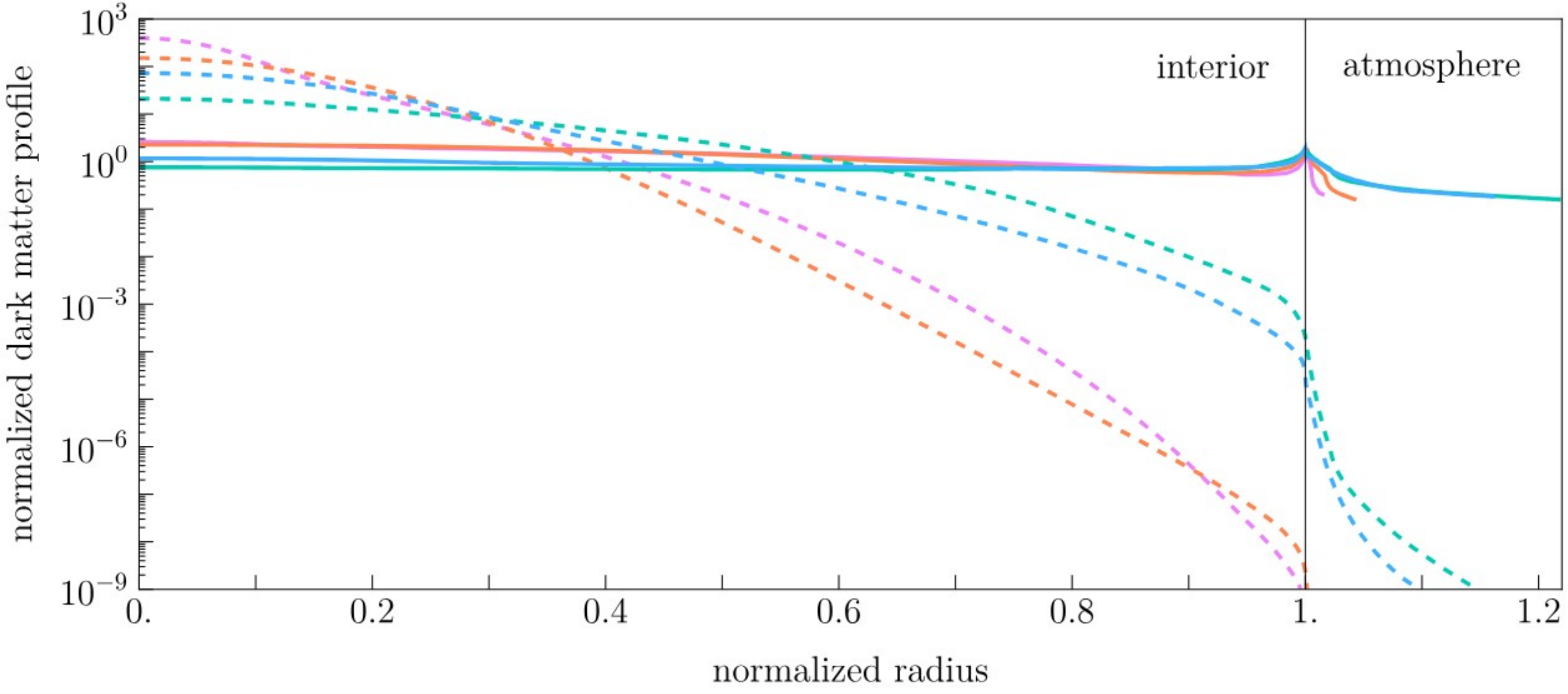


Figure 3. Dark matter radial profile in the Solar System gas and ice giants as labelled, for a 0.1 GeV (full) and a 1 GeV dark matter particle. The distance to the planet cores are normalized by each planetary radius; values above 1 indicate the atmosphere.

Jupiter: the IR signal

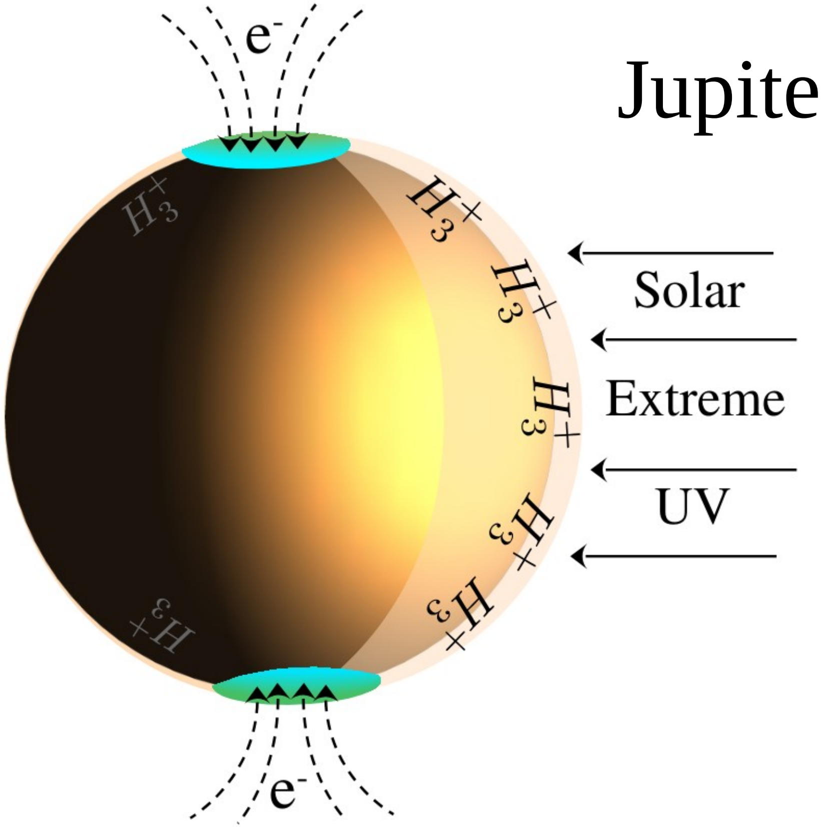


Figure 1. Schematic of H_3^+ production in Jupiter. Auroral H_3^+ emission near the magnetic poles is sourced by precipitating electrons, and solar extreme UV irradiates the day side and dominates H_3^+ production near the equator. No H_3^+ is expected from known processes at low latitudes on the night side, making it an ideal dark matter signal region.

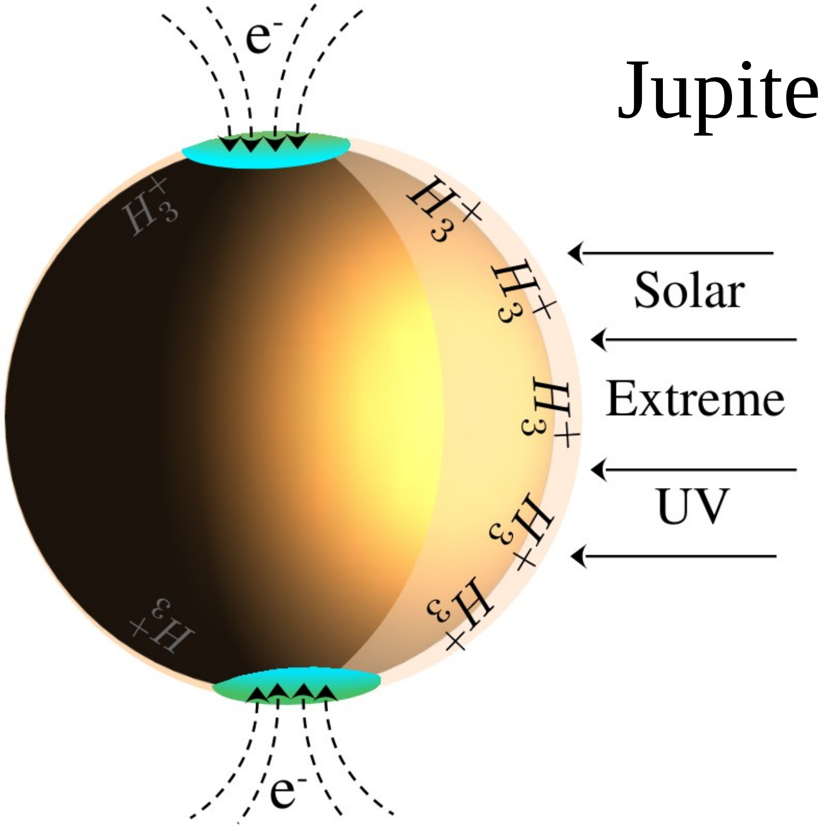
Ionizing radiation generates H_3^+

$$H_2 + e^{-*} \rightarrow H_2^+ + 2e^-$$

$$H_2^+ + H_2 \rightarrow H_3^+ + H$$

H_3^+ radiates extremely efficiently in the IR. It is Jupiter's *thermostat*.

Jupiter: the IR signal



Night-side Intensity

$$I^{H_3^+} < 0.03\ \mathrm{mW/m^2/\mu m/sr}$$

Day-side Intensity

$$I^{H_3^+}_{\mathrm{day}} = 0.09\ \mathrm{mW/m^2/\mu m/sr}$$

Day-side Ionizing Power

$$P^{\mathrm{EUV}}_{\mathrm{ion}} = 62\ \mu\mathrm{W/m^2}$$

Night-side Ionizing Power

$$P^{\mathrm{night}}_{\mathrm{ion}} < \frac{I^{H_3^+}_{\mathrm{max}}}{I^{H_3^+}_{\mathrm{day}}} \times \frac{E_{\mathrm{mol}}(T_{\mathrm{day}})}{E_{\mathrm{mol}}(T_{\mathrm{night}})} \times P^{\mathrm{EUV}}_{\mathrm{ion}} \times 1.5$$

$$P^{\mathrm{night}}_{\mathrm{ion}} < 40 \pm 17\ \mu\mathrm{W/m^2}$$

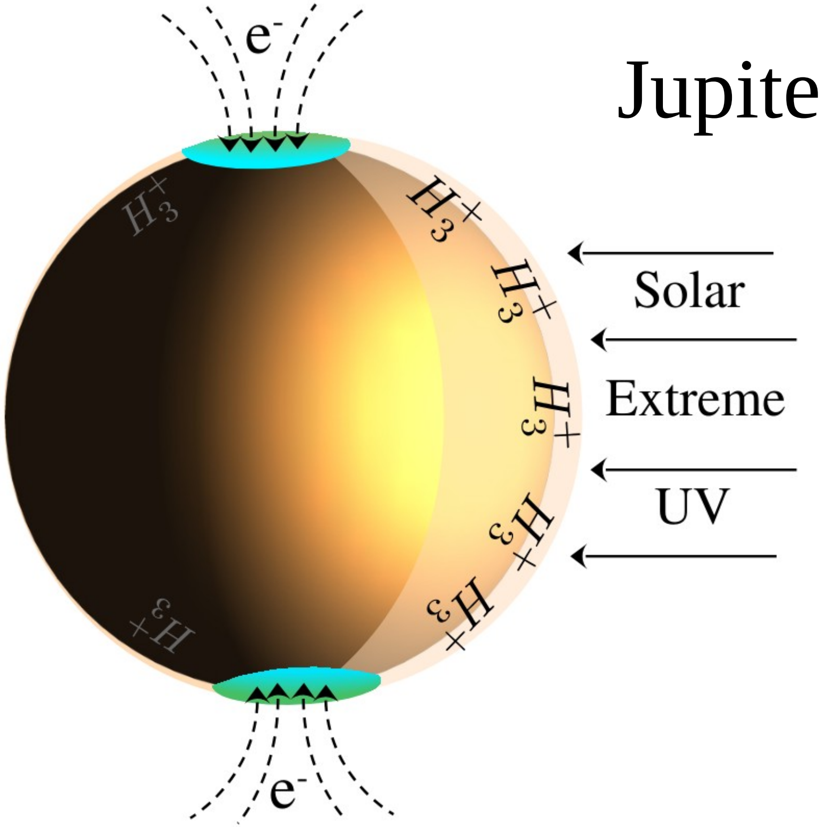
H_3^+ IR emission intensity is linear in ionizing power

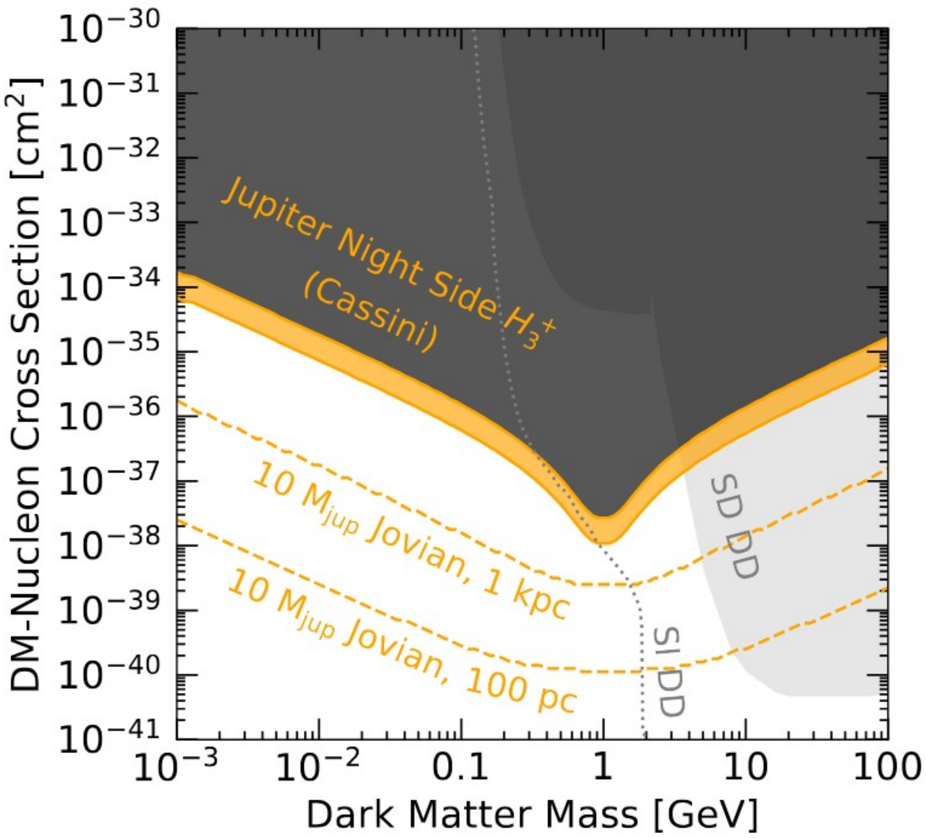
$$I^{H_3^+} = \alpha \times \beta \times P_{\mathrm{ion}} E_{\mathrm{mol}}(T)$$

Efficiency and geometric factors

Molar emissivity

Jupiter: the IR signal





Jupiter: the UV signal

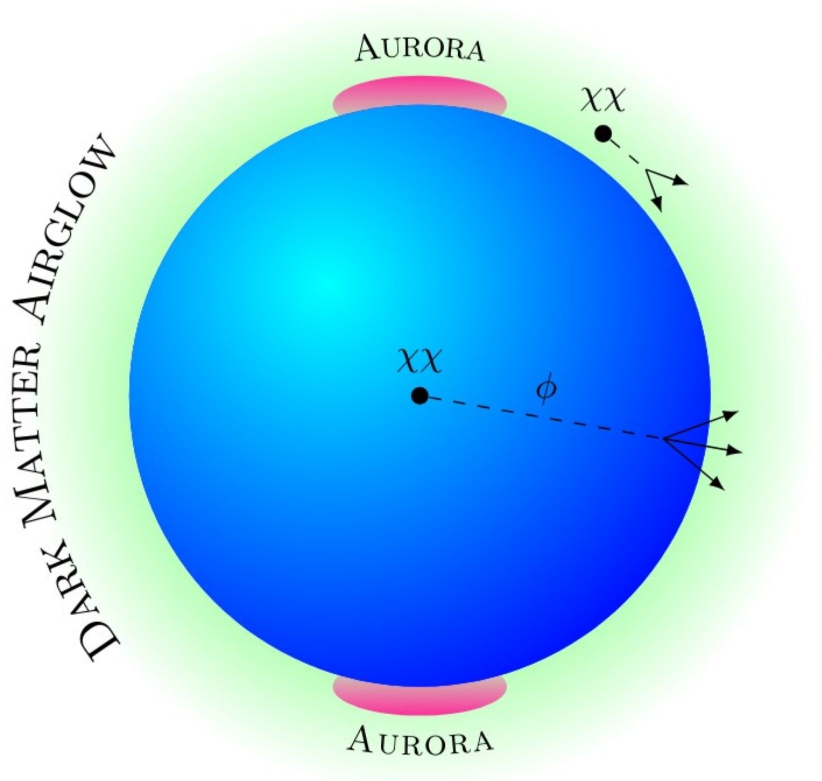


Figure 1. A planet with aurorae (at the poles, magenta), and a dark matter induced ultraviolet airglow (isotropic, green).

Ionizing radiation generates excited H_2

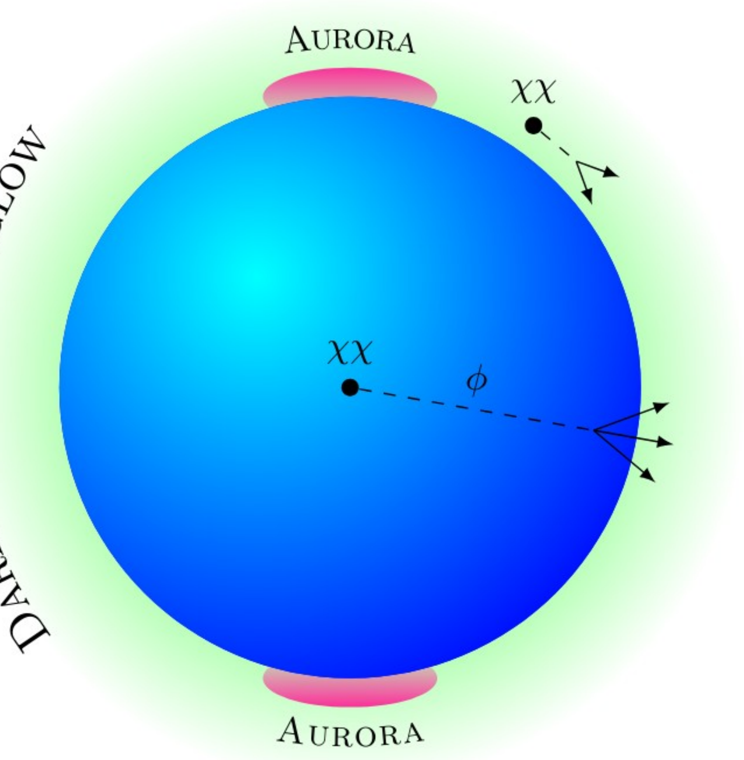
Ground state — Excited state

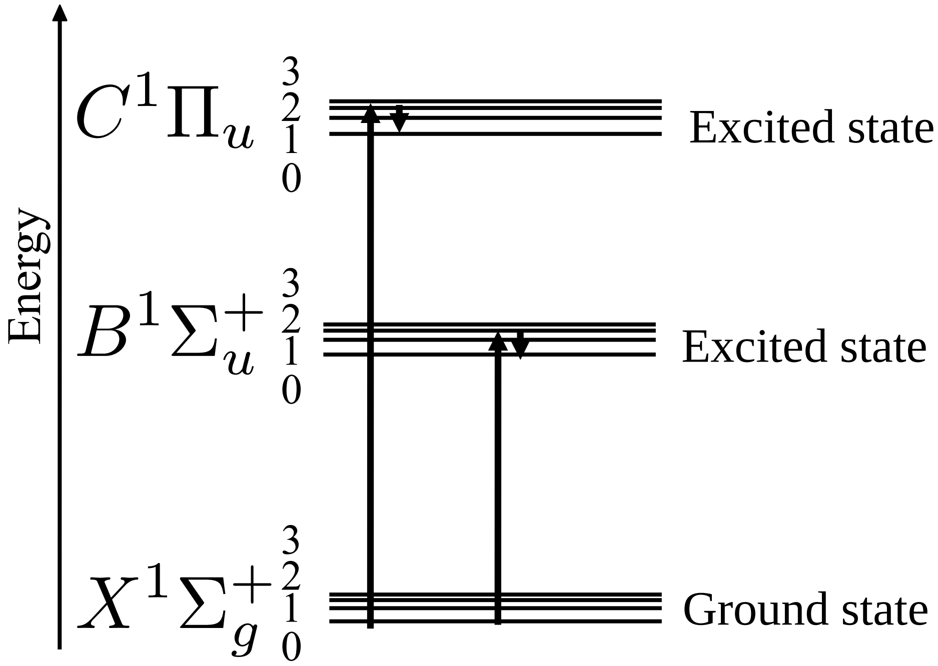
$$e^- + \mathrm{H}_2(X^1\Sigma_g^+) \rightarrow e^- + \mathrm{H}_2(B^1\Sigma_u^+)$$

Ground state — Excited state

$$e^- + \mathrm{H}_2(X^1\Sigma_g^+) \rightarrow e^- + \mathrm{H}_2(C^1\Pi_u)$$

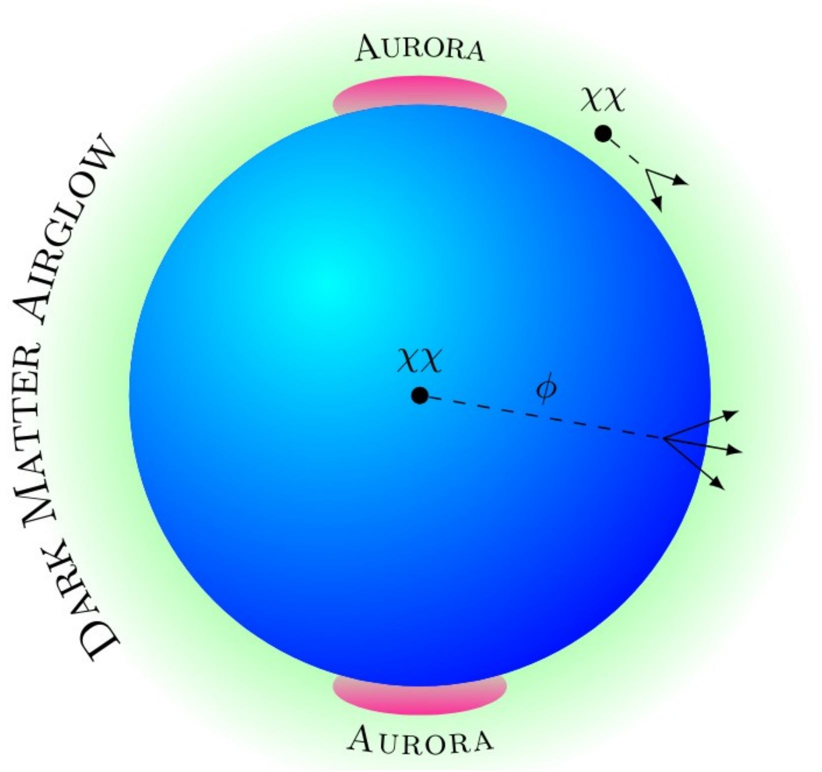
Jupiter: the UV signal



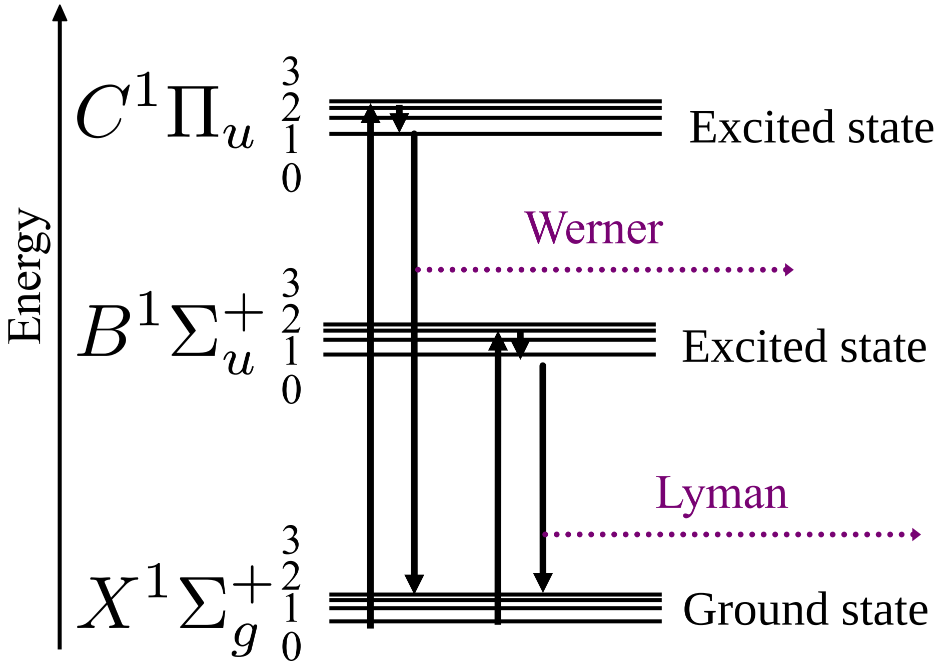


Collisions with charged particles drive excitations

Jupiter: the UV signal



Singlet excited states have short lifetimes τ ~ ns.



Radiative UV deexcitation
(Following collisional excitation)

Jupiter: the UV signal

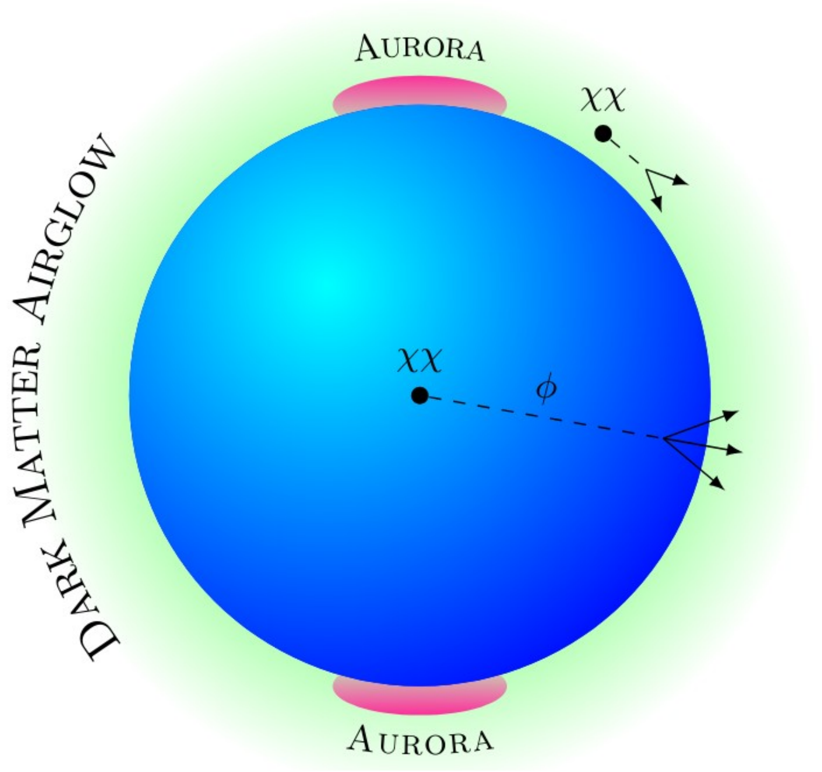
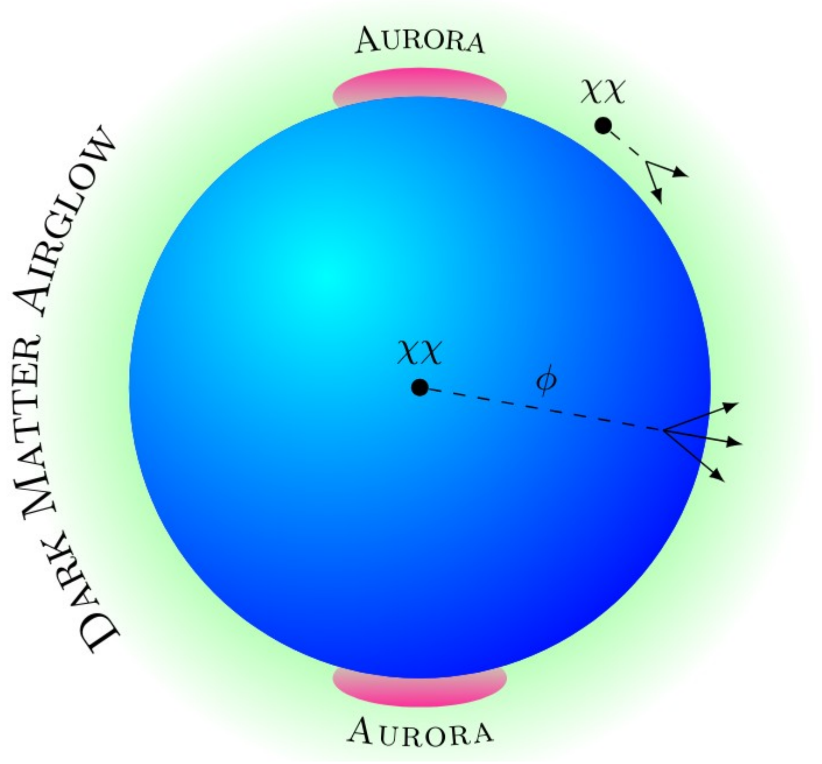


Table I. Measurements of the H_2 Lyman and Werner flux from the nightside equator region of the Solar System's giant planets, and corresponding input power into the planet's upper atmosphere. Uranus and Neptune's flux includes the Rydberg bands from H_2 and may originate from the dayside.

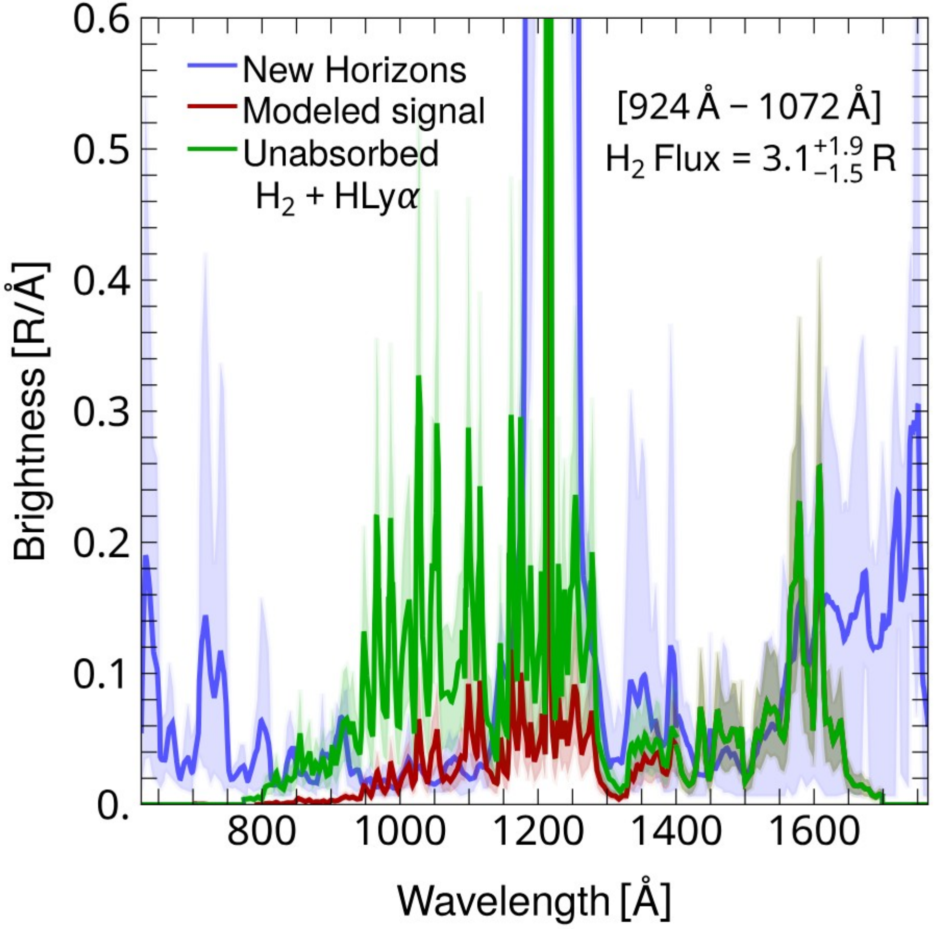
Planet	Flux [R]	Power [μW/m^2]	Space Probe	Ref.
Jupiter	$3.1^{+1.9}_{-1.5}$	$0.31^{+0.19}_{-0.15}$	New Horizons	[22]
Saturn	< 10	< 1	Voyager 1	[13]
Uranus	46	4.6	Voyager 2	[24]
Neptune	19 ± 3	1.9 ± 0.3	Voyager 2	[24]

10 R in H_2 UV surface brightness corresponds to about 1μW/m^2 energy in precipitating electrons.

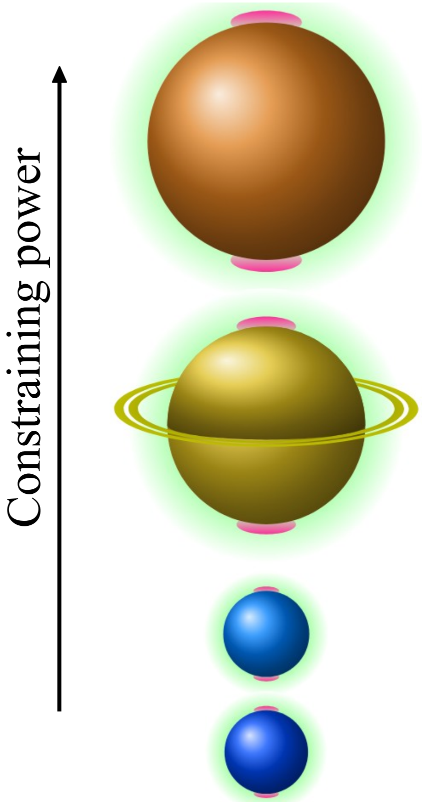
Jupiter: the UV signal



$$\text{Color Ratio} = \frac{\mathrm{I}(1550 - 1620\ \text{Å})}{\mathrm{I}(1230 - 1300\ \text{Å})} = 2.5$$



Constraining Spin-dependent Scattering

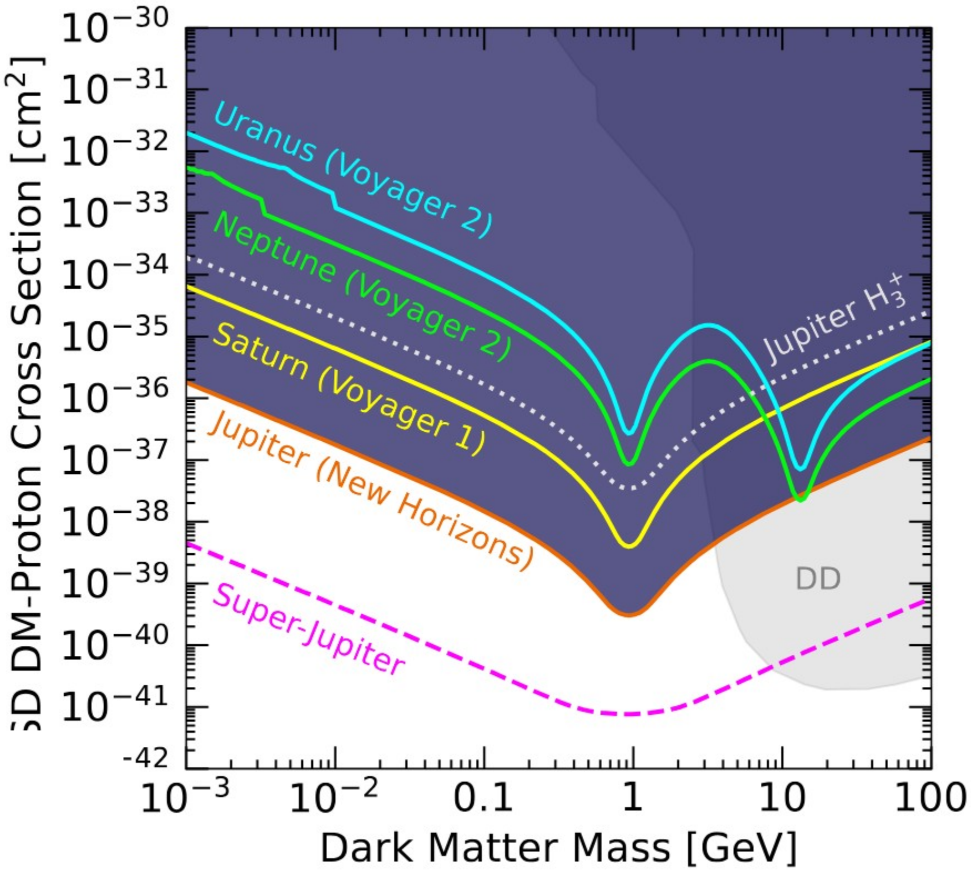


Jupiter

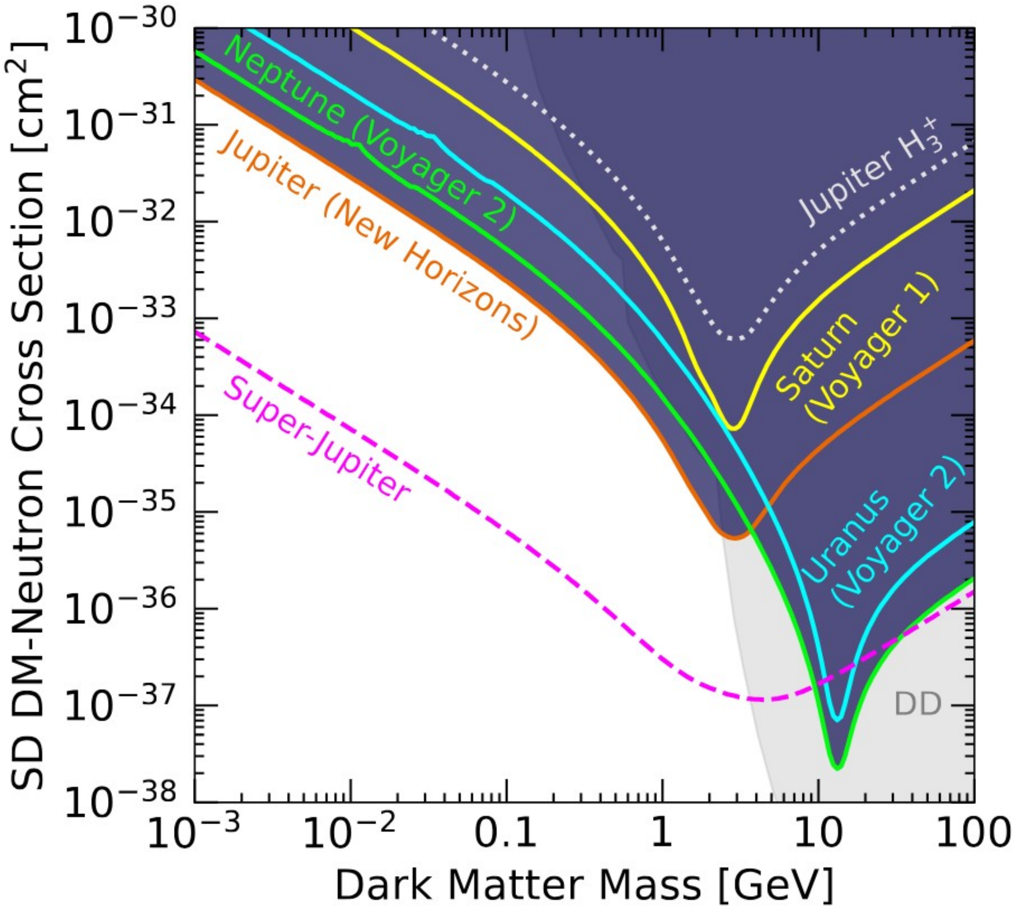
Saturn

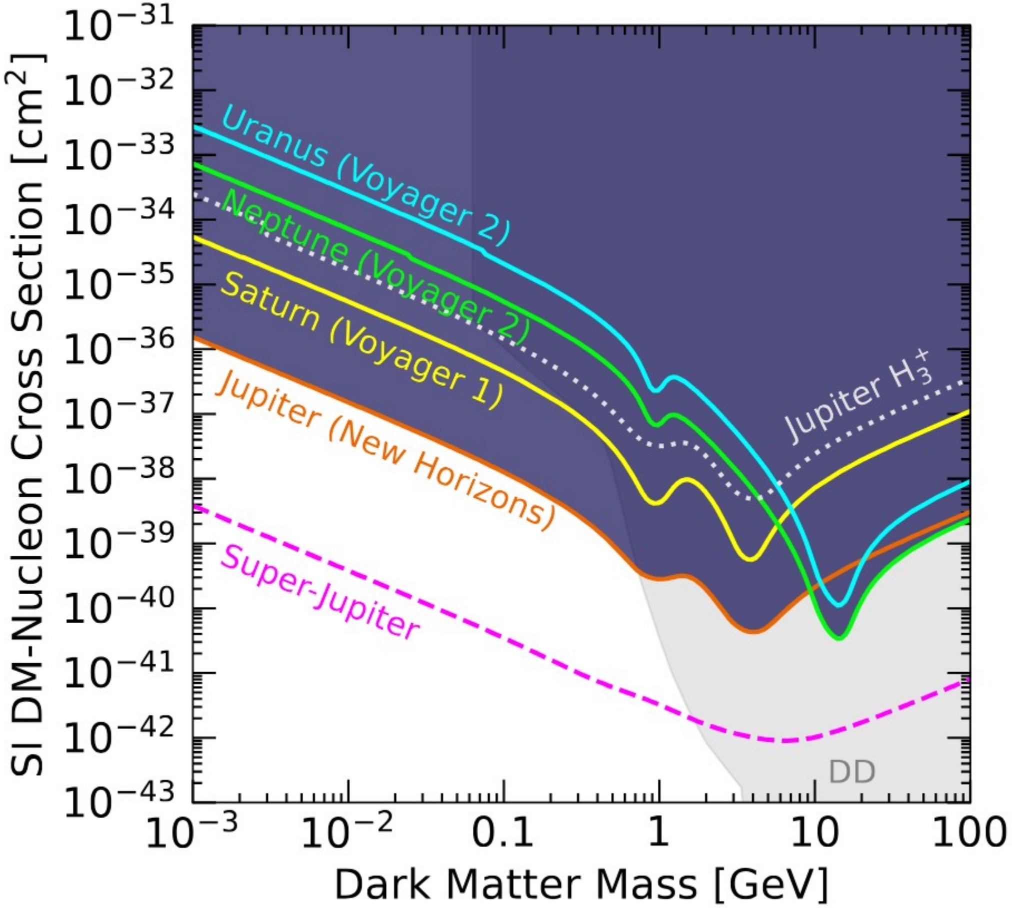
Neptune

Uranus



The UV signal





The UV signal - Teaser

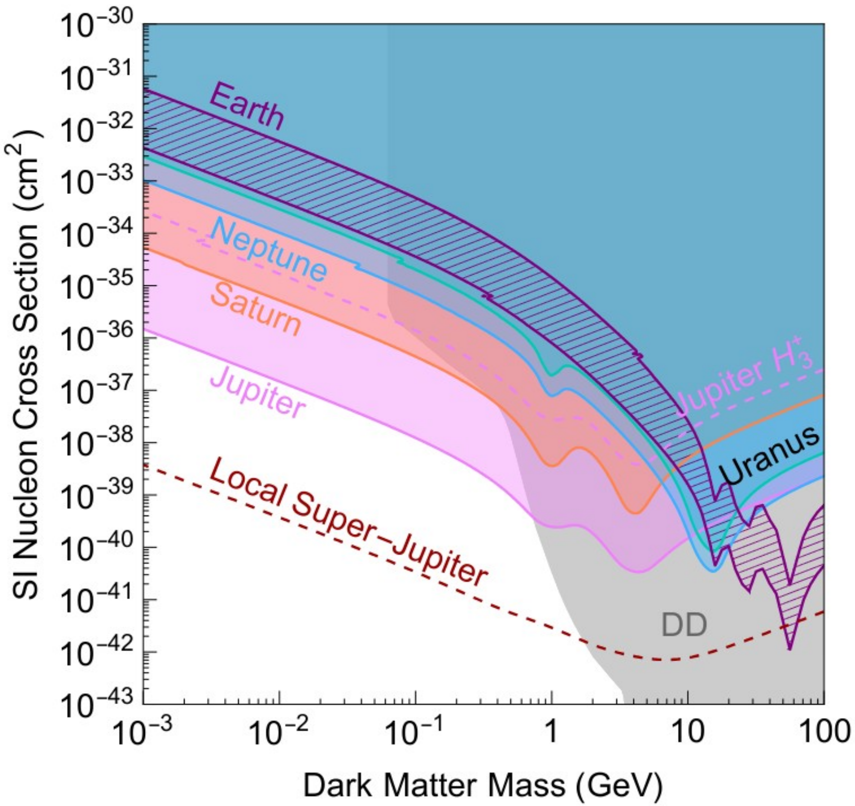


Figure 5. UV airglow limits on spin-independent dark matter interactions for the Solar System's giant planets, Earth, and a potential local Super-Jupiter, as labeled.