Direct & Indirect Detection of Dark Matter with Novel Targets: Why It Pays to Know a Chemist

CARLOS BLANCO
Our dark matter halo

Observations of our galaxy tell us:

Local dark matter density

$$\rho_{DM} = 0.4 \text{ GeV/cm}^3$$

Local dark matter velocity

$$\langle v_{DM} \rangle \approx 300 \text{ km/s}$$

Lighter masses → more particles

$$n_{DM} = \rho_{DM}/m_{DM}$$

More particles → larger fluxes

$$\phi_{DM} \sim v_{DM} n_{DM}$$
Detection pathways

Axions
Effective changes to Maxwell’s Eqs in radio frequency cavities

$10^{-22}$ eV
1 eV
1 keV
1 GeV
1 TeV

$M_{Pl} = 10^{19}$ GeV

Canonical WIMPs
Rare but energetic tracks in cryogenic detectors.

Ultra-heavy DM
Macroscopic tracks in old target material

eV-scale Bosons
Atomic excitations in e.g. Xenon

“Sub-GeV” DM
Feeble recoils
Single-quanta transitions

Wave-like
Particle-like

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Direct detection

\[ \bar{R}_{\text{sig}} \sim \xi \phi_{\text{DM}} \sigma \gtrsim \bar{R}_{\text{bkg}} \]

\[ \xi : \text{Signal generation efficiency} \]

What we need is:
- Small threshold energies
- Large signal efficiencies
- Low backgrounds

\[ \sigma_{\min} \gtrsim \bar{R}_{\text{bkg}} / \phi_{\text{DM}} \xi \]

Benchmark gives right DM abundance

Excluded

Freeze-out or Freeze-in

\[ m_{\text{DM}} \text{ [GeV]} \]

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Sub-GeV direct detection

$10^{-22}$ eV  1 eV  1 keV  1 GeV  1 TeV

$M_{Pl} = 10^{19}$ GeV

eV-scale Bosons & “Sub-GeV” DM
Classically allowed absorption & Inelastic scattering in *molecules* and *nanomaterials*

Kinetic energy of the dark matter

$\Delta E \sim 10^{-6} m_\chi \approx \mathcal{O}(\text{eV}) \left( \frac{m_\chi}{1 \text{ MeV}} \right)$

Imparted momentum in *scattering*

$|q| \sim m_\chi v_\chi \approx \mathcal{O}(\text{keV}) \left( \frac{m_\chi}{1 \text{ MeV}} \right)$

Imparted energy and momentum in *absorption*

$|q| \approx 0, \Delta E = m_\chi \left( \mathcal{O}(\text{eV}) \right)$

$\Psi_i(R, r) \rightarrow \Psi_f(R, r)$

$R$ : Nuclear coordinates

$r$ : Electron coordinates

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Interaction Rate

Rate “spectrum” (events in detector)

\[
\frac{dR}{d \ln E_r} \sim \int \frac{d^3 q}{q} \eta(v) |F_{DM}(q)|^2 |f_i \rightarrow f(q)|^2
\]

Mean inverse velocity (Astro)

\[
\eta(v)
\]

Transition form factor (Condensed matter / Chemistry)

\[
f_i \rightarrow f(q) = \langle \Psi_f | e^{i \vec{q} \cdot \vec{r}} | \Psi_i \rangle = \langle \tilde{\Psi}_f(k + q) | \tilde{\Psi}_i(k) \rangle
\]

Dark matter form factor (Particle physics)

\[
F_{DM}(q) = \begin{cases} 
1 & \text{, Contact interaction} \\
\left( \frac{\alpha m_e}{q} \right)^2 & \text{, Long-range interaction}
\end{cases}
\]
Electron Recoil: Photon Signal

Electron scattering or bosonic absorption leads to an excitation that decays via radiative emission.

A small unit that de-excites by emitting a photon is called a *chromophore*.

Electrons in crystals (exciton generation)

\[ |\psi_i(r)\rangle \sim u_v(r)e^{ik \cdot r} \quad |\psi\rangle^* \sim u_c(r)e^{ik \cdot r} \]

Excite from valence to conduction

Electrons in molecules and atoms

\[ |\psi_i\rangle \sim \psi_{lca}(r) \quad |\psi\rangle^* \sim \psi_{lca}^*(r) \]

Excite quantized levels
Carbon: a natural candidate

SP$_3$ – Hybrid Orbitals (Single Bonds)

$\sigma$-bond

Ex : C$_3$H$_8$

Single bonded backbone is rigid

SP$_2$ – Hybrid Orbitals (Double Bonds)

$\pi$-bond

Ex : C$_3$H$_6$

Systems of double-bonds make de-localized “fluorescent” states

The de-localized p-orbital networks of carbon-based molecules are natural DM detector candidates

$$q_e \approx 1/a_0 \sim \mathcal{O}(\text{keV})$$

$$|q| \sim m_X v_X \approx \mathcal{O}(\text{keV}) \left( \frac{m_X}{1 \text{ MeV}} \right)$$
Fluorescence with DM

Characteristic fluorescence spectra of chromophores

Probability for the photon to free-stream

$$\Phi_{FB} \sim (1 - a_{xx})$$

What we need is:
Large detectable signal efficiencies

Chromophore:

Solid molecular crystals:
$$\Phi_{FB} \approx 65\%$$
A pilot experiment

Problem: describe the interaction between DM (BSM) with molecules (chemistry)

Build the many body wave functions from molecular orbitals

\[
\Psi_G = |\psi_2 \bar{\psi}_2 \psi_1 \bar{\psi}_1 \psi_1 \bar{\psi}_1| \\
\Psi_i^j = \frac{1}{\sqrt{2}} (|\psi_1 \bar{\psi}_1 \cdots \psi_i \bar{\psi}_j \cdots \psi_N \bar{\psi}_N| - |\psi_1 \bar{\psi}_1 \cdots \psi_j \bar{\psi}_i \cdots \psi_N \bar{\psi}_N|)
\]

Compute the molecular form factors

\[
f_i(q) = \int d^3p \bar{\psi}_n(p) \bar{\psi}_n^{*}(p + q)
\]

Para-xylene (EJ-301)

Molecular scintillators are cheap, well characterized, and extremely clean.

[CB, Collar, Kahn, Lillard ‘19: 1912.02822]
First Experimental Setup

[CB, Collar, Kahn, Lillard: 1912.02822]
Results: EJ-301

(Contact interaction)  (Long-range interaction)

About 6 months from theory development to results!

[CB, Collar, Kahn, Lillard: 1912.02822]
Now what we need is:

Lower background

Option 1
Reduce background in the absorption step, i.e. selective excitation.

*Molecular crystals* have fundamentally anisotropic excitation probabilities. This leads to daily modulating signals from DM.

Option 2
Reduce background in the emission step, i.e. selective signal generation.

*Quantum dots* can produce a pair of time-coincident photons following excitation.
The earth experiences a dark matter “wind” in the direction of travel around the Milky Way.

Change in relative orientation between detector and dark matter wind leads to *daily* modulation.
Trans-Stilbene

De-localized and planar network of double bonds

Molecular planes oriented in crystal lattice

Large optical-quality crystals

Carman, et.al. ’18 (J. of Crystal Growth)
Daily Modulation

Predicted rate changes by up to 70% throughout the day.
That’s a verifiable signal!

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

[CB, Kahn, Lillard, McDermott: 2103.08601]
Interaction Rate

Rate “spectrum” (events in detector)
\[
\frac{dR}{d \ln E_r} \sim \int \frac{d^3 \vec{q}}{q} \eta(v)|F_{DM}(q)|^2 |f_i \rightarrow f(q)|^2
\]

Mean inverse velocity (Astro)
\[\eta(v)\]

Transition form factor (Condensed matter / Chemistry)
\[f_i \rightarrow f(q) = \langle \Psi_f | e^{i \vec{q} \cdot \vec{r}} | \Psi_i \rangle = \langle \tilde{\Psi}_f(k + q) | \tilde{\Psi}_i(k) \rangle\]

Dark matter form factor (Particle physics)
\[F_{DM}(q) = \begin{cases} 
1, \quad \text{Contact interaction} \\
\left( \frac{\alpha m_e}{q} \right)^2, \quad \text{Long-range interaction}
\end{cases}\]
Sensitivity & Reach

(Contact interaction)

(Long-range interaction)

Modulating signals improve sensitivity by about two orders of magnitude and provide the potential for discovery.

*1kg of t-stilbene can probably be found within a few blocks of this room.
Inelastic scattering or bosonic absorption on nuclear states leads to an excitation that decays via radiative emission.

\[ \Delta E \sim \mathcal{O} \text{(few eV)} \left( \frac{m_\chi}{100 \text{ MeV}} \right)^2 \left( \frac{m_N}{130 \text{ GeV}} \right)^{-1} \]
Ionizing through nuclear recoil: Atoms

The **Migdal effect** in atoms has been invoked in e.g. Xenon to extend the sensitivity of noble liquid detectors to lower masses.

Initial nuclear recoil

Nucleus recoils faster than motion of electrons

Electronic transition to ionized state

\[
|\psi_i\rangle \sim e^{i\frac{mq}{MN}} \vec{q} \cdot \vec{r} \psi_{AO}(r_\beta)
\]

\[
v = \frac{q}{MN}
\]

\[
f_{i \rightarrow f} \approx \frac{m_e}{M_N} \vec{q} \cdot \langle \vec{r} \rangle_{i \rightarrow f}
\]

Migdal transition probability is suppressed by kinematic mis-match.
The Molecular Migdal Effect(s)

Center of mass recoil (CMR) effect
Caused by center of mass motion

COM recoil effect is the molecular analog of the semiclassical Migdal effect

\[ P_{CMR} \sim \frac{m_e}{M_{mol}} \]
Suppressed by kinematic factor due to moving the whole molecule.

Non-adiabatic coupling (NAC) effect
Caused by relative motion

NAC caused by effects beyond Born-Oppenheimer approximation

\[ P_{NAC} \sim \frac{m_e}{M_N} \]
Suppressed by kinematic factor due to moving a single atom.

Blanco ‘22: 2208.09002
Si rate is calculated using the CMR-equivalent Migdal effect. Is there an NAC-equivalent in Si?

Center of mass recoil effect is predicted to be subdominant at all masses.

Non-adiabatic coupling effect is predicted to dominate due to favorable kinematic factor.

Simplest molecular models already competitive. Is there an optimal molecular target?

[CB, Harris, Kahn, Lillard, Perez-Rios: 2208.09002]
Persistent daily modulation at large dark matter mass is generically predicted for the molecular Migdal effects. We predict that the same class of molecules that make good directional detectors for electron scattering will also be ideal for nuclear scattering because of the directional molecular Migdal effects.
Finding optimal targets for NAC

Molecules with vanishing transition dipole moments are classically forbidden from absorbing. However, a deformation in the molecular structure can generate a dipole, i.e. a measurable NAC-induced absorption!

\[ \epsilon \sim \langle \psi_f (r; R) | \vec{r} | \psi_i (r; R) \rangle |_{R \neq R_0} \neq 0 \]

That’s classically forbidden by symmetry

Recall that photon absorption is proportional to the transition dipole moment.

\[ \epsilon \sim \langle \Psi_f | \vec{r} | \Psi_i \rangle = 0 \]

Non-adiabatic form factor is asking about how the electrons respond to nuclear deformation.

\[ f_{e,NAC} \sim \langle \psi_f | \nabla R | \psi_i (r) \rangle \]
Finding optimal targets

Problem: Chemical space is unreasonably large

How many molecules can be made with only 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

We need a method to:
1. Look for favorable properties - cheminformatics
2. extra(intra)polate onto new molecules – machine learning

UV Absorption spectrum of toluene
ML for DM Direct Detection

Method:
1. Learn the latent space of molecules → Property prediction
2. Generate new molecules by optimizing for properties in lower dimensional space.

Machine learning can do both of these

How many molecules can be made with only C, O, N, F, & H?

- 9 atoms: 100s of Thousands (Complete dataset– QM9)
- 30 atoms: 100s of Billions (Sparse data)

Validate on QM9 then apply interpolator to larger set

[CB, Smirnov, Cook: 2401.xxxxx]
Fluorescence with DM Works

Now what we need is:

Lower background

Option 1
Reduce background in the absorption step, i.e. selective excitation.

*Molecular crystals* have fundamentally anisotropic excitation probabilities. This leads to daily modulating signals from DM.

Option 2
Reduce background in the emission step, i.e. selective signal generation.

*Quantum dots* can produce a pair of time-coincident photons following excitation.
What are Quantum Dots?

Quantum confinement affects the long-wavelength physics

\[ R \rightarrow \infty \text{ nm} \]

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

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

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

\[ E(k) \]

\[ \Delta E_g \]

\[ \Delta E_{QD} > \Delta E_g \]

Zherebetsky et al., Science 344, 1380 (2014)
Quantum Dots

- **Absorption**: Creation of a “hot” exciton – an electron/hole pair with energy significantly larger than the bandgap

- **Non-Radiative Transition**: Multi-exciton generation when energy is greater than twice the bandgap creates several band-edge excitons.

- **Emission**: Radiative recombination of several band-edge excitons producing several coincident photons

[CB, Essig, Fernandez-Serra, Ramani, Slone: 2208.05967]
PbS Quantum Dots

(Contact interaction)  (Long-range interaction)

Essentially background free @ this scale

Assuming a realistic dark rate for the photodetectors, QD-based detectors using existing technology would be deployed and easily scaled to overtake existing limits.

[CB, Essig, Fernandez-Serra, Ramani, Slone: 2208.05967]
PbS QDs

In the case of eV-scale dark photon absorption, we can use existing data to predict the sensitivity of QD-based detectors.

Key conclusions of QD analysis

1) The interaction rate in a semiconductor generated by DM is the same if the semiconductor is monolithic or nanoscopically disperse.

2) In a QD-based experiment, the readout is independent of the target.

3) The signal can be tuned through control of quantum confinement.

[CB, Essig, Fernandez-Serra, Ramani, Slone: 2208.05967]
LETTER OF INTENT:
QUAntum dot Dark matter Recoil detection with Abalone photosensors (QUADRA)

Carlos Blanco$^{1,2}$, Jan Conrad$^2$, Rouven Essig$^3$, Alfredo Davide Ferella$^5$, Tim Linden$^2$, Jörn Mahlstedt$^2$, and Val Zwiller$^4$

$^1$Department of Physics, Princeton University, Princeton, NJ 08544, USA
$^2$Stockholm University and The Oskar Klein Centre for Cosmoparticle Physics, Alba Nova, 10691 Stockholm, Sweden
$^3$C. N. Yang Institute for Theoretical Physics, Stony Brook University, USA
$^4$Department of Applied Physics, Royal Institute of Technology, Roslagstullsbacken 21, 114 21 Stockholm, Sweden
$^5$Department of Physics and Chemistry, University of L’Aquila, 67100 L’Aquila, Italy and INFN-Laboratori Nazionali del Gran Sasso and Gran Sasso Science Institute, 67100 L’Aquila, Italy

October 31, 2022
Deployment

\[ R \sim R_{\text{PMT}} + \delta R \]

\[ R_{2\gamma-QD} \lesssim \Delta TR_{\text{PMT}}^{3/2} \]

![Diagram of deployment setup](image)
Beyond direct detection

We can use the same theoretical techniques that we’ve developed to predict rates in astrophysical objects.
Beyond direct detection

We can use the same theoretical techniques that I’ve developed to predict rates in detectors to predict rates in astrophysical objects.
Dark matter in Molecular Clouds

Very dense and cold molecular clouds are almost entirely opaque.
\[ n_{\text{H}_2} \sim O(10^2) \text{cm}^{-3} \]

Ionization from CR produces ionization fraction: \( \zeta^{\text{H}_2} \)

\[ \text{CR} + \text{H}_2 \rightarrow \text{CR} + \text{H}_2^+ + e^- \]

This is well measured through astro-spectroscopy of tracer molecules (line intensity measurements)

However, DM annihilation into ionizing SM particles can also produce ionized fraction

\[ \zeta_{i}^{\text{H}_2} = 2\pi \int \frac{dN_i}{dE}(E)\sigma_i(E)dE \]

[Prabhu, CB: 2211.05787]
Dark matter in Molecular Clouds

Constraints on DM w/ ultra-light mediator from dense (black) and diffuse (blue) molecular clouds. The hatched region represents the uncertainty in our bounds coming from the uncertainty in the inferred CR ionization rate due to gas depletion onto grain surfaces.

There would otherwise be an open window of parameter space where the dark matter is too strongly-coupled to be visible even by satellite experiments.

[Prabhu, CB: 2211.05787]
Dark matter in Molecular Clouds

Molecular cloud ionization (Thick lines) can constrain almost all remaining parameter space for a strongly-coupled leptophillic subcomponent of DM which would never make it to other detectors.

The Molecular Migdal effect(s) in space

Molecular cloud ionization (Thick lines) can constrain almost all remaining parameter space for a strongly-coupled leptophillic subcomponent of DM which would never make it to other detectors.
Conclusions

1) We have done an extremely effective job looking for WIMPs, now we must look beyond.

2) By developing the formalism that describes the interaction between dark matter and molecules or nano-materials, we can propose detection strategies capable of delving deep and searching wide across the dark matter parameter space.

4) This remains one of the few ways to probe high-energy physics at the bench-top scale.

5) Future hybrid methods may bring together both strategies giving multiplicative improvements to sensitivity.
Acknowledgements

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QDs – Cheap, tunable and scalable

Φ dependence on the solution concentration for 3nm and 3.3nm PbS QDs in toluene.

\[ n_e \sim 10^{20} \text{ cm}^{-3} = 10^{23} \text{ L}^{-1} \]
Strongly Confining Quantum Dots

Semiconducting nano-spheres

\[ E_{\text{confinement}} = \frac{\hbar^2 \pi^2}{2a^2} \left( \frac{1}{m_e} + \frac{1}{m_h} \right) = \frac{\hbar^2 \pi^2}{2\mu a^2} \]

\[ E = E_{\text{bandgap}} + E_{\text{confinement}} \]

\[ = E_{\text{bandgap}} + \frac{\hbar^2 \pi^2}{2\mu a^2} \]

\[ E_{\text{kin}} \sim \frac{1}{r^2} \]

\[ E_{\text{coulomb}} \sim \frac{1}{r} \]
Fluorescence: Binary Scintillators

- Solvent: Primary target starts the signal
- Solute: Dilute fluor gets the signal out of the bulk

Intensity

Energy

Absorption

Emission

arXiv: 1912.02822
PbS QDs: Improvements

"Blind" mode

\[ R_{\text{PMT}} \sim 10\text{Hz} \]

"Active" mode

\[ R \approx R_{\text{PMT}} + \delta R + R_{\gamma-QD} \]

\[ R_{\gamma-QD} \lesssim \sqrt{R_{\text{PMT}}} \]
PbS QDs: Improvements

\[ R_{\text{coinc}}^0 \approx \Delta T R_{\text{PMT}}^2 \]

\[ R_{\text{coinc}} \approx \Delta T R_{\text{PMT}}^2 + 2\Delta T R_{\text{PMT}} \delta R + R_{2\gamma-QD} \]

\[ R_{2\gamma-QD} \lesssim \Delta T R_{\text{PMT}}^{3/2} \]
PbS QDs: Optimism for comparison

DM-Electron Scattering (no background 1-photon signal)

Blanco '22: 2208.05967

Carlos Blanco November 27 2023
Daily Modulation: Small Mass

Molecular form factors and modulating rates for DM masses near threshold, \(m_\chi = 2\) MeV. In the contour plots, the gridded shaded regions indicate the kinematically accessible momentum transfers \(\vec{q}\) for the four molecules that comprise the unit cell of the crystal, shown at \(t = 0\) and \(t = 10\) h. Here, \(\vec{q}\) is given in the molecular basis, \(q_x = \vec{q} \cdot \vec{L}, q_y = \vec{q} \cdot \vec{M}\), and the kinematically accessible region is defined by \(v_-(\vec{q}) < v_{\text{esc}}\).

[CB, Kahn, Lillard, McDermott: 2103.08601]
Daily Modulation: Large Mass

Same as previous figure but for large DM masses, $m_\chi = 100$ MeV. Only the nearly-spherical region near $q \sim 0$ with inner boundary $q_{\text{min}} \simeq 1.6$ keV is kinematically forbidden. As a result, the daily modulation amplitude is smaller, driven by the anisotropy of the inner secondary peaks and the tails of the primary peaks.

[CB, Kahn, Lillard, McDermott: 2103.08601]
Electron Recoil: Charge Signal

Electron scattering

\[ \Delta E_r = \left( \frac{m_X^2}{m_T} \right) \times 10^{-6} \]

\[ \Delta E \sim \mathcal{O} \text{(few eV)} \left( \frac{m_X}{1 \text{ MeV}} \right)^2 \]

What has such transition energies?

- Semiconductor band gaps
- Maybe atomic ionization

Electrons in crystals (exciton generation)

\[ |\psi_i(r_{\beta})\rangle \sim u_v(r)e^{ik' \cdot r} \quad |\psi_f(r_{\beta})\rangle \sim u_c(r)e^{ik \cdot r} \]

Electrons in atoms (ionization)

\[ |\psi_i\rangle \sim \psi_{\text{STO}}(r_{\beta}) \quad |\psi_f\rangle \sim e^{ik \cdot r}, \quad r \gg a_0 \]
Semiconductor CCDs

Nuclear Recoil: Phonon Signal

\[ |\Psi_i\rangle = |0\rangle \quad \rightarrow \quad |\Psi_f\rangle = a^\dagger(k) |0\rangle \]

\[ \Delta E \sim \mathcal{O}\left(\text{few eV}\right) \left(\frac{m_\chi}{100 \text{ MeV}}\right)^2 \left(\frac{m_N}{130 \text{ GeV}}\right)^{-1} \]

\[ \omega \sim \mathcal{O}(10-100 \text{ meV}) \]
Calorimeters

Optical primary

Acoustic athermal Secondary

$N_{\text{acoustic}} \sim \mathcal{O}(100)$

$E_0 \sim 10 - 100 \text{ meV}$

Directional Targets: Polyacenes

Trans-Stilbene

\[ E_1 = 4.2 \text{eV} \]

Beveridge & Jaffe '65

Dipole allowed \( E_1 \)!
## Trans-Stilbene

<table>
<thead>
<tr>
<th>$s$</th>
<th>Platt Symbol</th>
<th>Symmetry</th>
<th>$\Delta E$ [eV]</th>
<th>Configuration amplitudes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$s_1$</td>
<td>$^1B$</td>
<td>$B_u$</td>
<td>4.240</td>
<td>$d_{7,8} = 0.94, \quad d_{4,11} = -0.24$</td>
</tr>
<tr>
<td>$s_2$</td>
<td>$^1G^-$</td>
<td>$B_u$</td>
<td>4.788</td>
<td>$d_{7,10} = 0.53, \quad d_{5,8} = 0.53, \quad d_{6,11} = 0.37, \quad d_{4,9} = -0.37$</td>
</tr>
<tr>
<td>$s_3$</td>
<td>$^1G^-$</td>
<td>$A_g$</td>
<td>4.800</td>
<td>$d_{7,9} = 0.53, \quad d_{6,8} = 0.53, \quad d_{5,11} = 0.37, \quad d_{4,10} = -0.37$</td>
</tr>
<tr>
<td>$s_4$</td>
<td>$^1(C, H)^+$</td>
<td>$A_g$</td>
<td>5.137</td>
<td>$d_{7,11} = 0.41, \quad d_{5,9} = -0.41, \quad d_{6,10} = -0.41, \quad d_{4,8} = -0.59$</td>
</tr>
<tr>
<td>$s_5$</td>
<td>$^1H^+$</td>
<td>$B_u$</td>
<td>5.791</td>
<td>$d_{7,11} = 0.54, \quad d_{6,9} = 0.54, \quad d_{7,12} = 0.33, \quad d_{3,8} = 0.33$</td>
</tr>
<tr>
<td>$s_6$</td>
<td>$^1G^+$</td>
<td>$A_g$</td>
<td>6.264</td>
<td>$d_{7,9} = 0.68, \quad d_{6,8} = -0.68$</td>
</tr>
<tr>
<td>$s_7$</td>
<td>$^1C^-$</td>
<td>$A_g$</td>
<td>6.013</td>
<td>$d_{7,11} = 0.66, \quad d_{4,8} = 0.54, \quad d_{5,8} = -0.65$</td>
</tr>
<tr>
<td>$s_8$</td>
<td>$^1G^+$</td>
<td>$B_u$</td>
<td>6.439</td>
<td>$d_{7,10} = 0.65$</td>
</tr>
</tbody>
</table>

Table 1: The first eight excited states $s_n=1...8$, with their energy eigenvalues $\Delta E(s_n)$ with respect to the ground state and coefficients $d_{ij}^{(n)}$ as calculated by Ting and McClure.

$$
|s_n\rangle = \sum_{i,j>i} d_{ij}^{(n)} |\psi_i^j\rangle,
\sum_{ij} |d_{ij}^{(n)}|^2 = 1.
$$

$$
f_{g\rightarrow s_n}(\vec{q}) = \langle \psi_{s_n}(\vec{r}_1 \ldots \vec{r}_{14}) | \sum_{m=1}^{14} e^{i\vec{q}\cdot\vec{r}_m} | \psi_G(\vec{r}_1 \ldots \vec{r}_{14}) \rangle
= \sum_{ij} d_{ij}^{(n)} \langle \psi_i^j | e^{i\vec{q}\cdot\vec{r}} | \psi_G \rangle
= \sqrt{2} \sum_{ij} d_{ij}^{(n)} \langle \Psi_j(\vec{r}) | e^{i\vec{q}\cdot\vec{r}} | \Psi_i(\vec{r}) \rangle.
$$
Same as previous figures (top) for a light mediator DM form factor $F_{DM} = (\alpha m_e / q)^2$. Here, the contour plots show $F_{DM}^2 |f(s_1)|^2$ which appears in the rate integrand; the scattering is dominated by the smallest kinematically-allowed $q$. **Top:** Molecular form factors with $q_z = 0$ and rate modulations for $m_\chi = 2$ MeV. **Bottom:** Molecular form factors with $q_z = 0$ and rate modulations for $m_\chi = 100$ MeV.
Local DM Phase Space
