

Atomic Response Functions for Light Dark Matter Direct Searches

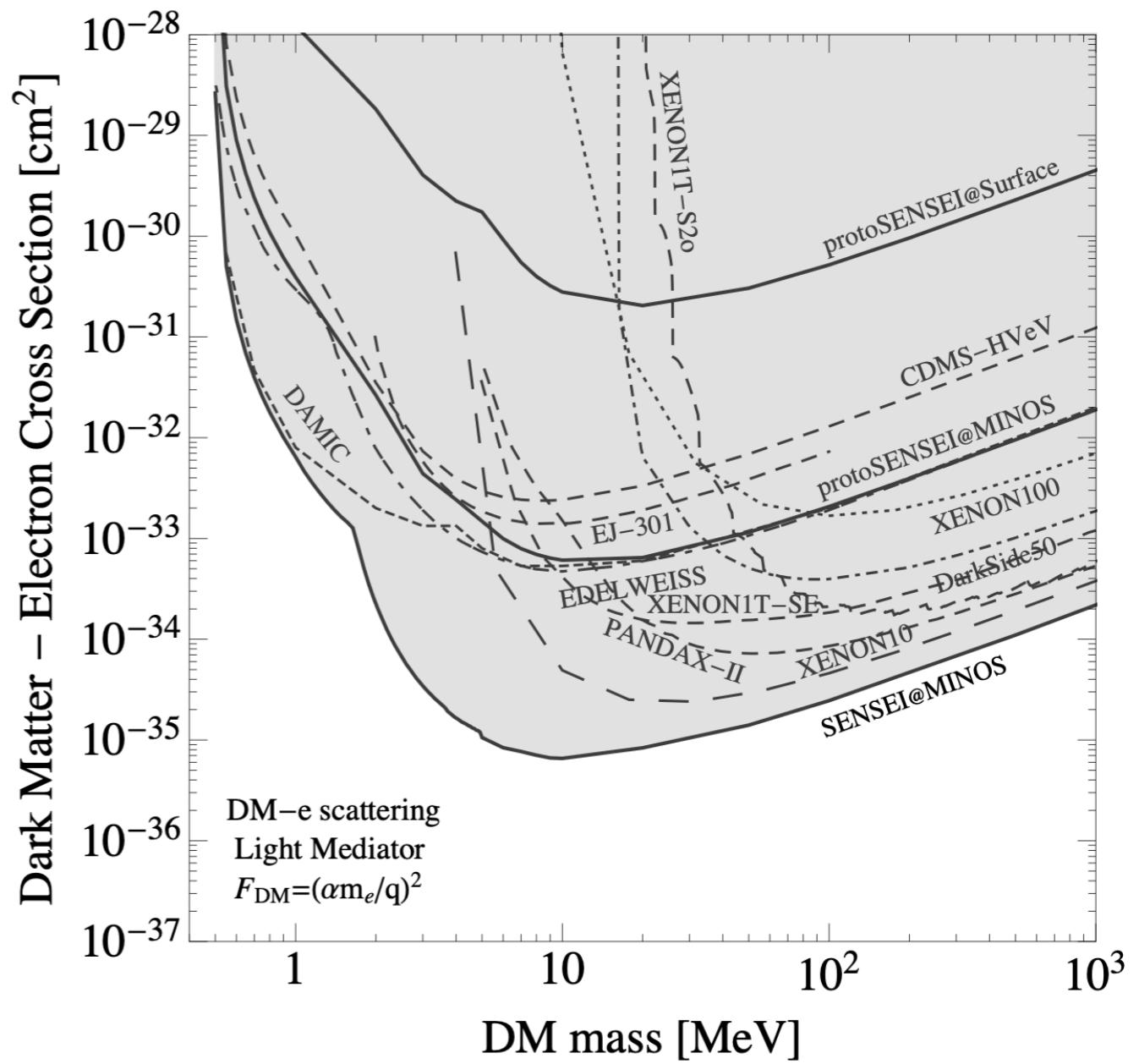
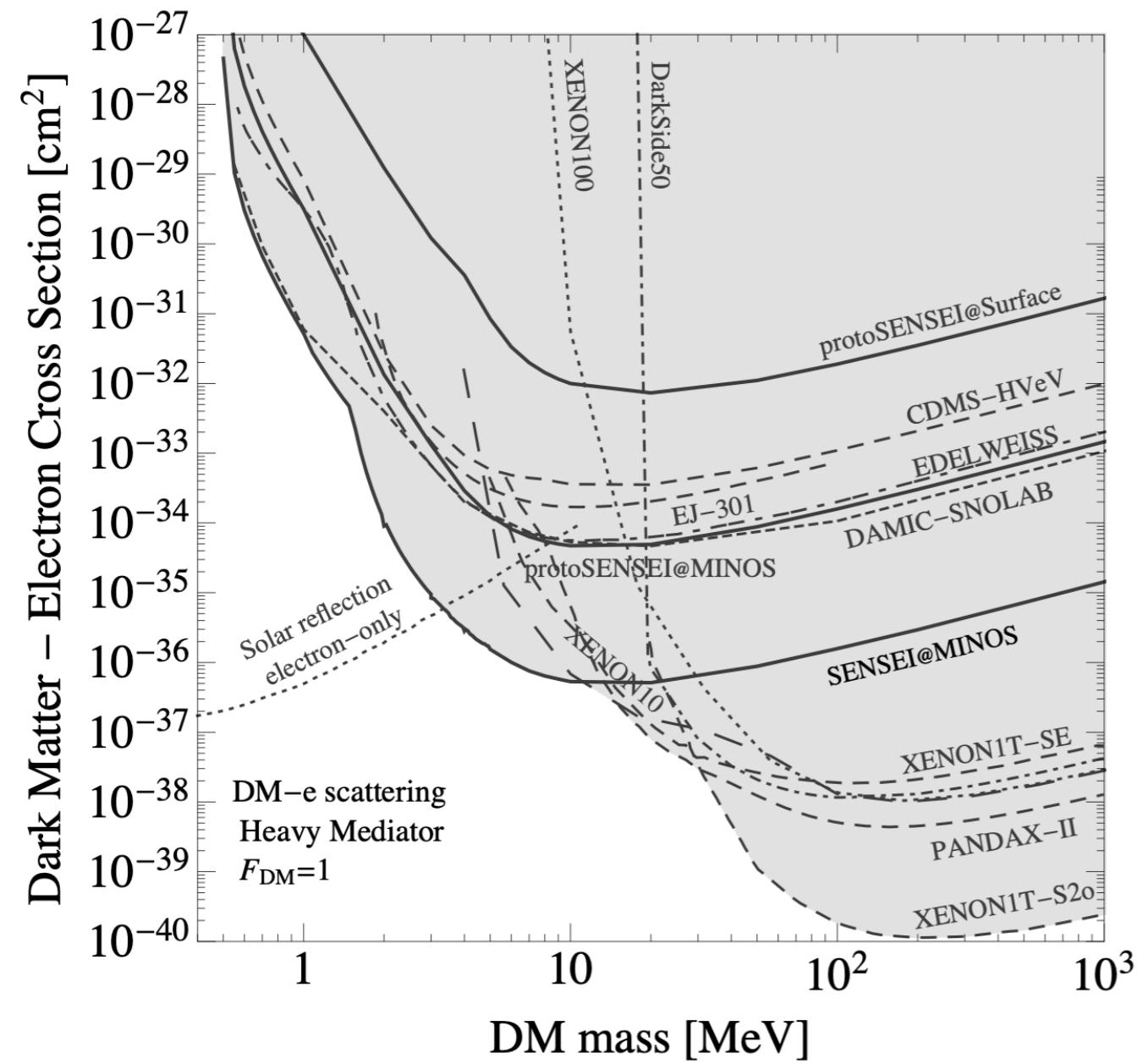
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Direct Searches of LDM

- Generically, m_χ in meV-GeV.
- When cold $v_\chi \sim 10^{-3}$, $q_{\max} \sim m_\chi v_\chi$ and $T_{\max} \sim m_\chi v_\chi^2$ (scattering) or m_χ (absorption).
- Detector thresholds: $T_{NR} \sim \text{keV}$, $T_{ER} < \text{keV}$, so sub-GeV direct searches mainly rely on ER, which can come from χe int. or Migdal effects via χN int.
- ER through atomic ionization: T in 10 eV - tens of keV.
- In condensed matter systems, regions of even smaller T are actively pursued.

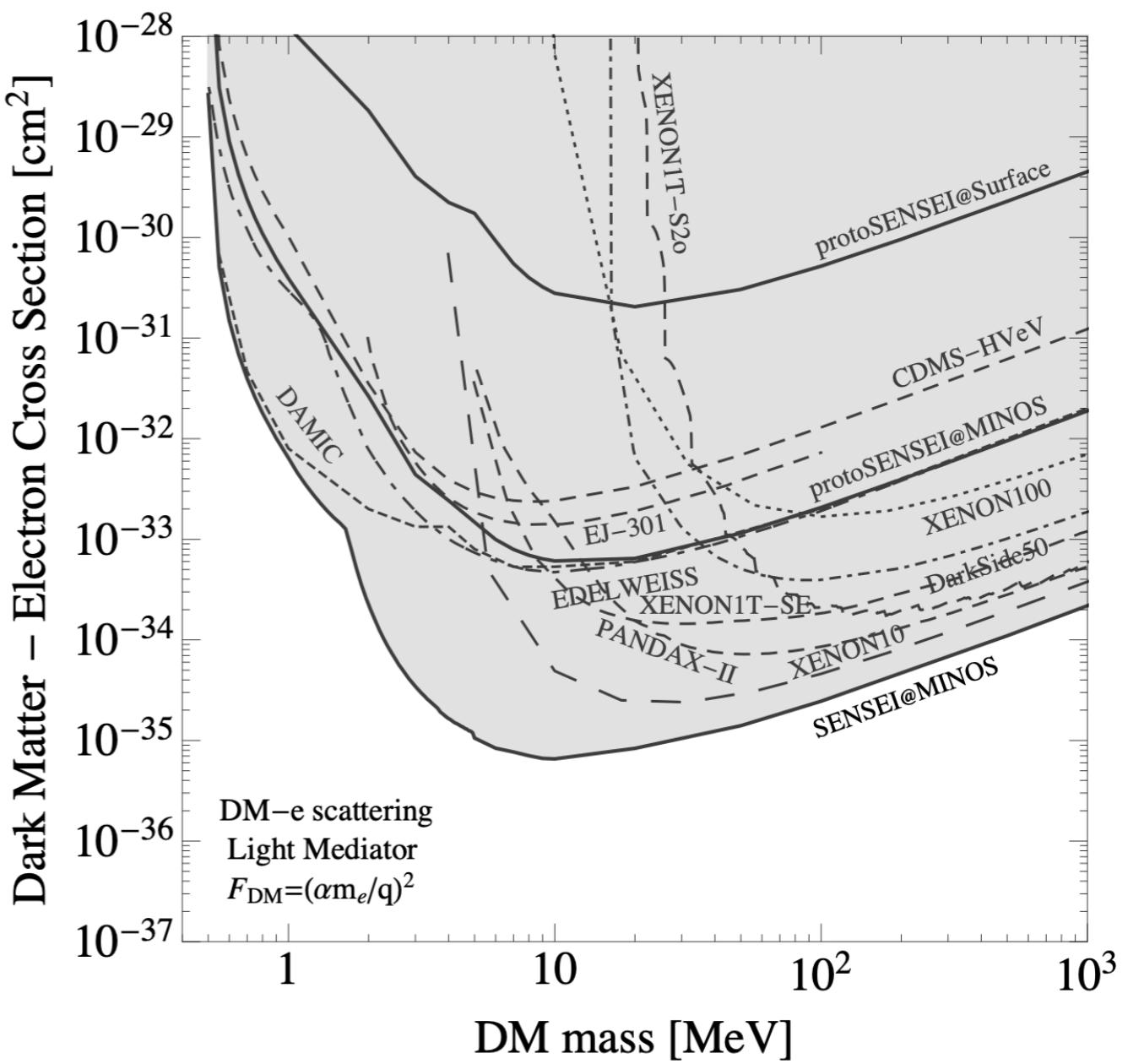
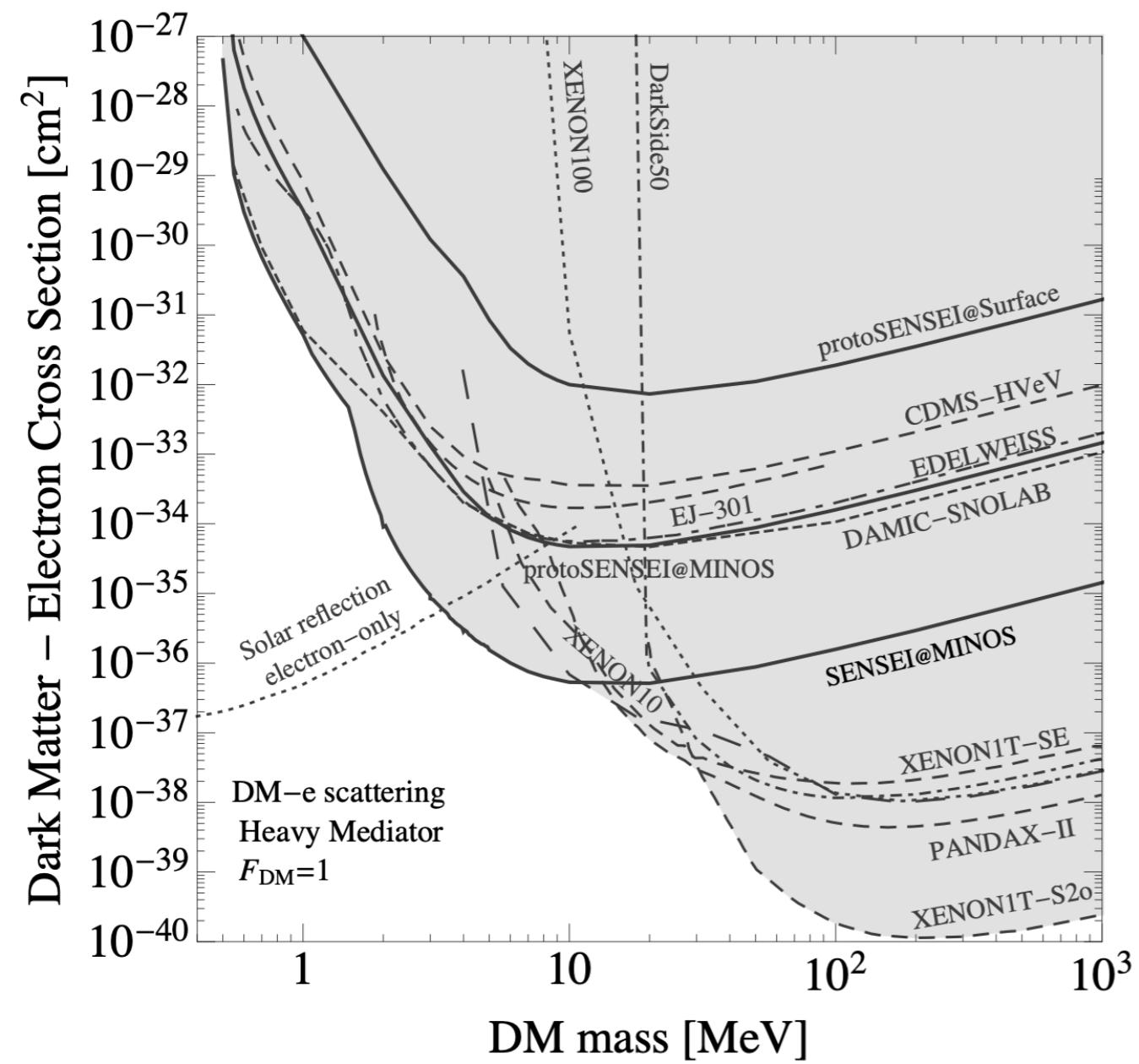
Exclusion Limits: Null Results Viewed Positively



arXiv:2203.08297

The landscape of low-threshold dark matter direct detection in the next decade

Exclusion Limits: How Reliable They Are?



arXiv:2203.08297

The landscape of low-threshold dark matter direct detection in the next decade

Counting Rate dR/dT : Where Theory Enters

- AstroP./Cosmo.: DM velocity spectrum

$$\frac{dR}{dT} = n_\chi \int d^3v_\chi f(\vec{v}_\chi) v_\chi \frac{d\sigma}{dT}$$

- HEP: DM-matter interaction (model-driven / EFT)

$$\begin{aligned}\mathcal{L}_{\chi e}^{(\text{LO})} = & (c_1 + d_1/q^2) \chi^\dagger \chi e^\dagger e \\ & + (c_4 + d_4/q^2) \chi^\dagger \vec{s}_\chi \chi \cdot e^\dagger \vec{s}_e e\end{aligned}$$

- NP/AMP/CMP: Differential cross section

$$\begin{aligned}\frac{d\sigma}{dT} = & \frac{1}{2\pi v_\chi^2} \int_{q_{\min}}^{q_{\max}} q dq \left\{ (c_1 + d_1/q^2)^2 \mathcal{R}_{\text{SI}}(T, q) \right. \\ & \left. + \frac{1}{12} s_\chi (s_\chi + 1) (c_4 + d_4/q^2)^2 \mathcal{R}_{\text{SD}}(T, q) \right\}\end{aligned}$$

Response Functions: Where MB Physics Hides

Contains the full dynamical information of how a complex
MB system reacts to external perturbation

$$\mathcal{R}_O(T, \vec{q}) = \sum_F \sum_I \left| \langle F | \hat{O}(\vec{q}) | I \rangle \right|^2 \delta(E_F - E_I - T)$$

- Operator \hat{O} is prescribed by the DM interaction
- For unpolarized scattering, $\vec{q} \rightarrow q$.
- Biggest challenge: MB wave functions for the initial, $|A\rangle$, and the final $|A^+, e^-\rangle$ states.
- For certain (\hat{O}, T, q) , possible to extract from experiments.
 - Single atom Migdal effect through σ_γ [CPL et al., PRD 102, 121303(R) (2020)]
 - DM-cond. through dielectric function [Hochberg et al., PRL 127, 151802 (2021)]

Several Approaches Been Applied

	QEdark ^[1]	DarkARC ^[2]	Our past work ^[3,4]
Ground state (s.p. orbitals)	<ul style="list-style-type: none"> Roothaan Hartree-Fock (RHF) 	<ul style="list-style-type: none"> Roothaan Hartree-Fock (RHF) 	<ul style="list-style-type: none"> Multi-configuration Dirac-Fock (MCDF)
Excitation (continuum, transition matrix)	<ul style="list-style-type: none"> Solved by potential extracted from RHF 	<ul style="list-style-type: none"> Hydrogen-like w.fs. by RHF s.p. energies 	<ul style="list-style-type: none"> Frozen-core approximation (FCA)
Relativistic correction?	No	No	Yes
Residual correlation?	No	No	No

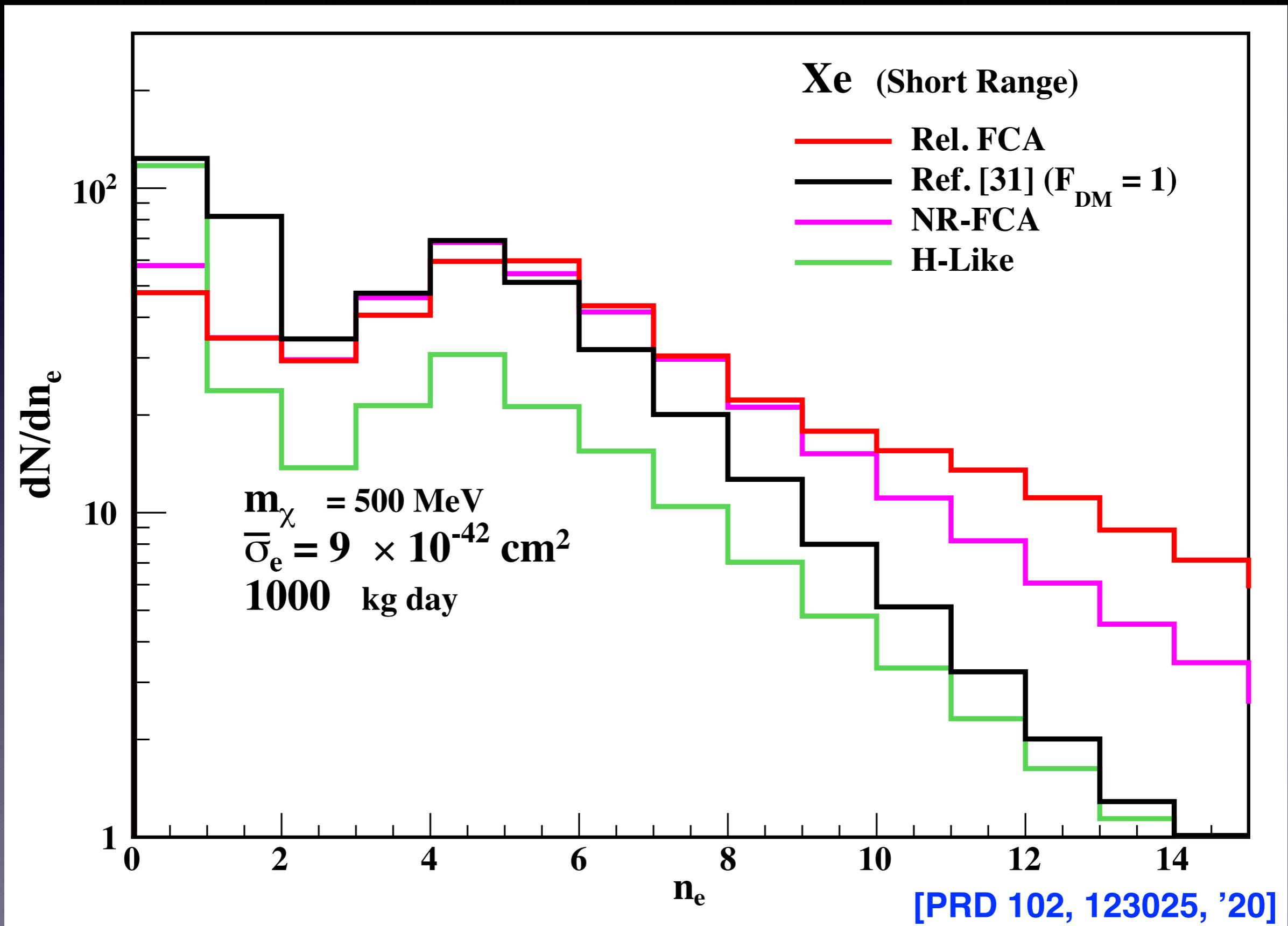
[1] Essig et al., PRD 96, 043017 (2017)

[2] Catena et al., PRR 2, 033195 (2020) [similarly, Agnes et al. (DarkSide), PRL 121, 081307 (2018)]

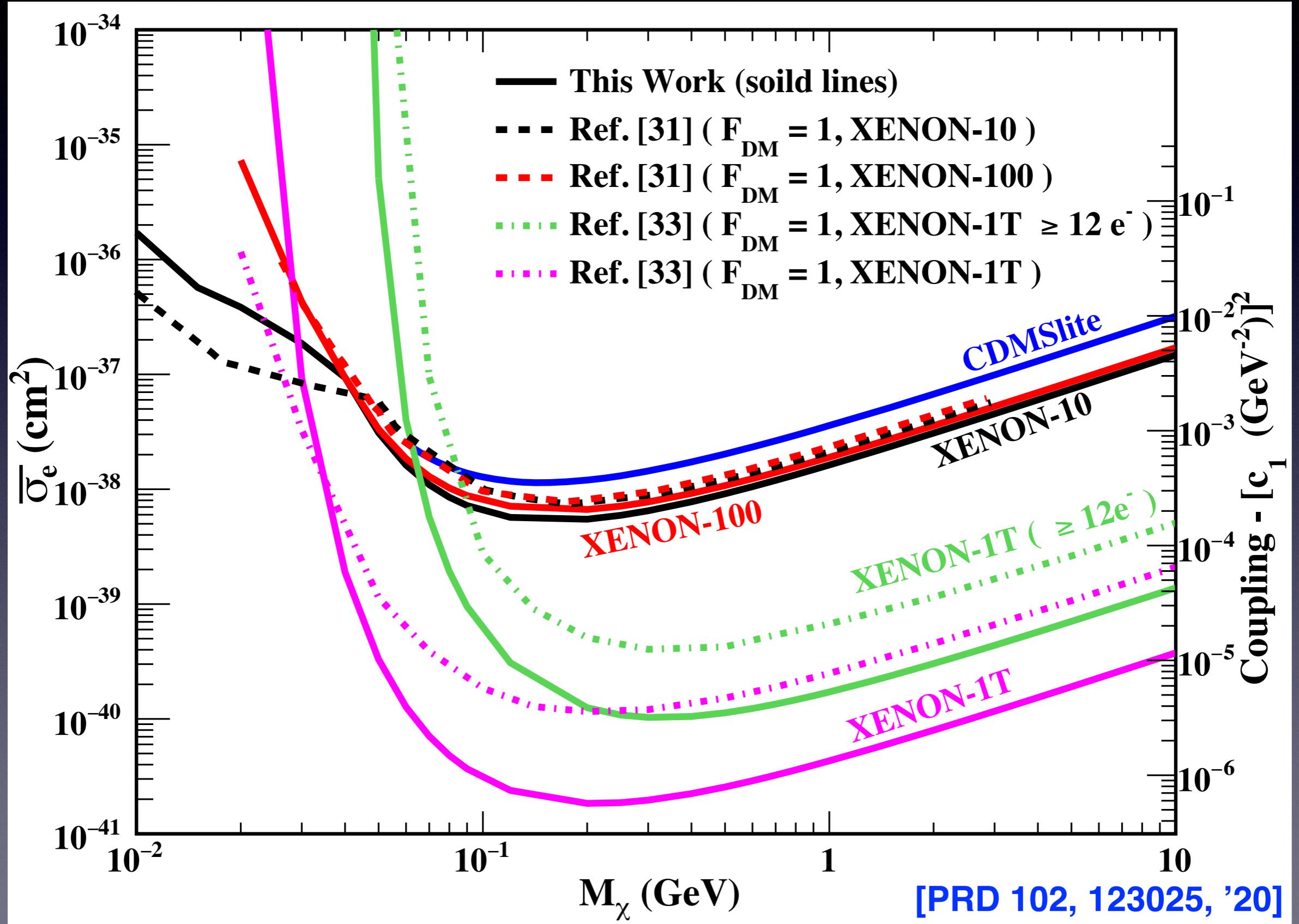
[3] Pandey, ..., CPL et al., PRD 102, 123025 (2020) [similarly Roberts et al., PRD 100, 063017 (2019)]

[4] CPL et al., PRD 106, 063003 (2022)

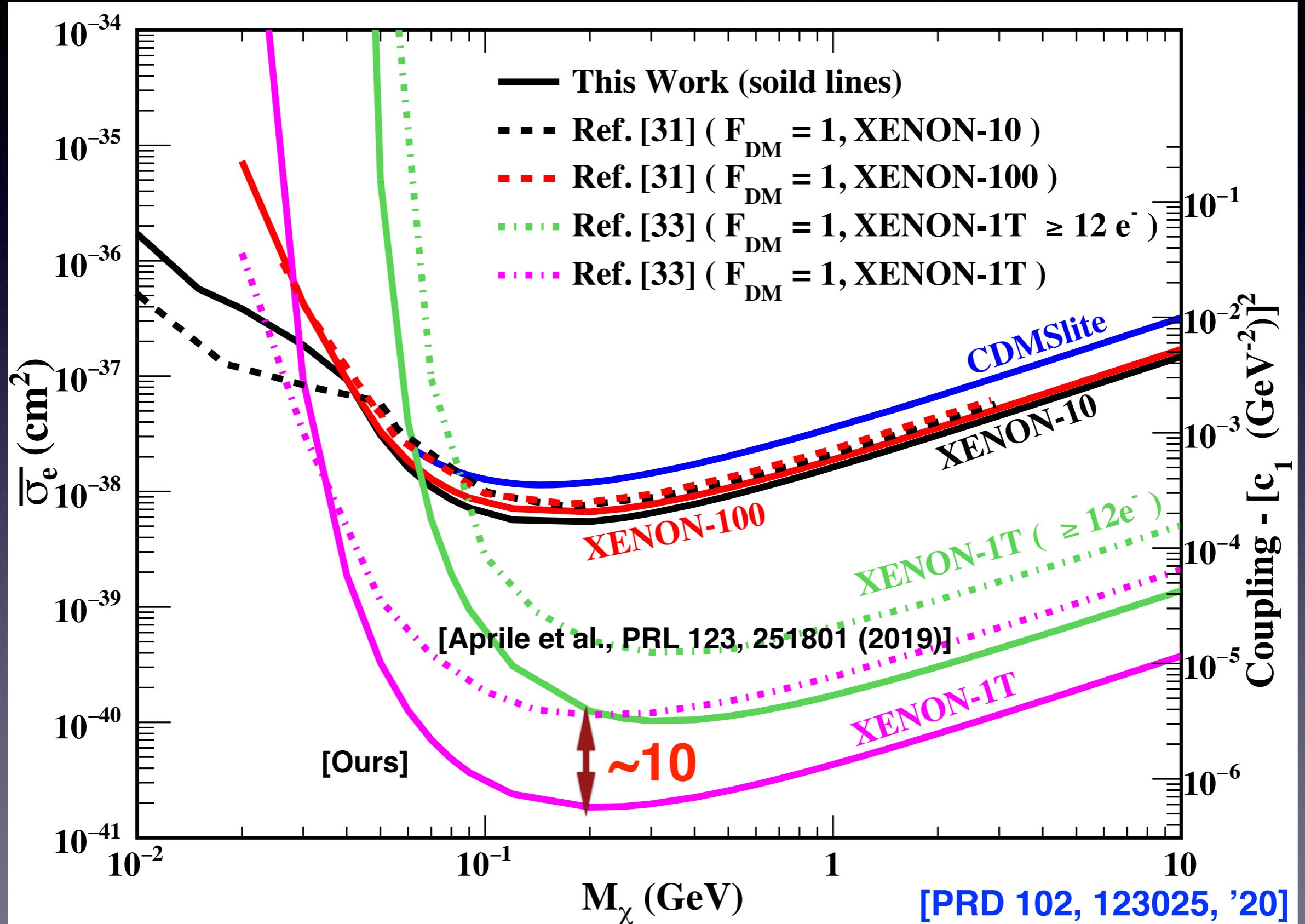
Predictions Differ!



Impact on the Exclusion Plot



Impact on the Exclusion Plot



Our New Work (in progress)

	QEdark	DarkARC	Our new work
Ground state (s.p. orbitals)	<ul style="list-style-type: none">• Roothaan Hartree-Fock (RHF)	<ul style="list-style-type: none">• Roothaan Hartree-Fock (RHF)	<ul style="list-style-type: none">• Multi-configuration Dirac-Fock (MCDF)
Excitation (continuum, transition matrix)	<ul style="list-style-type: none">• Solved by potential extracted from RHF	<ul style="list-style-type: none">• Hydrogen-like w.fs. by RHF s.p. energies	<ul style="list-style-type: none">• MC relativistic RPA (MCRPA) in full
Relativistic correction?	No	No	Yes
Residual correlation?	No	No	Yes

MCDF + MCRRPA

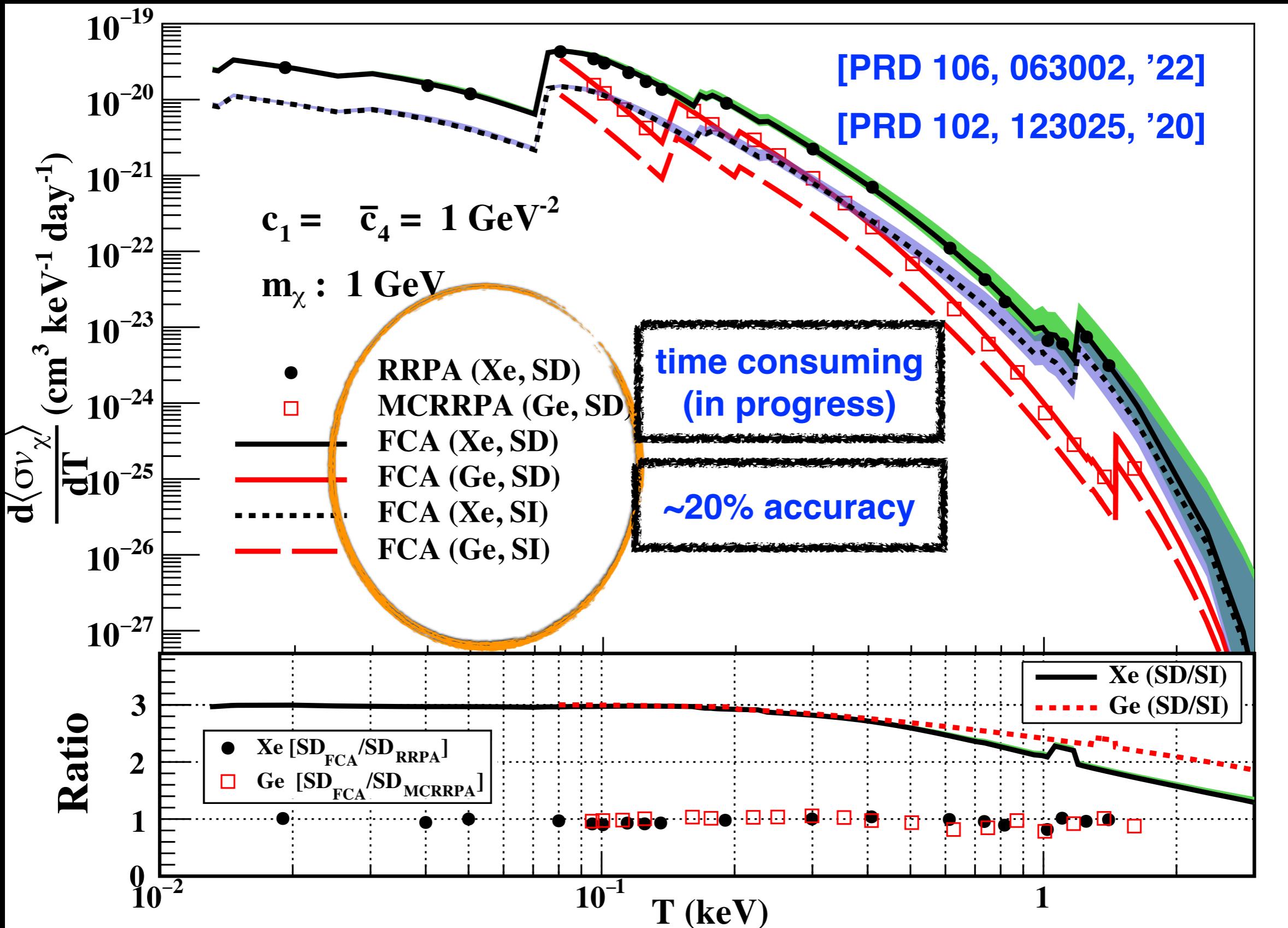
An *ab initio* method improved upon Hartree-Fock theory

- MC [multi-configuration]: open-shell atoms have more than one ground-state configuration. E.g., for Ge:

$$|J = 0\rangle = c_1 |[\text{Zn}]4p_{1/2}^2\rangle + c_2 |[\text{Zn}]4p_{3/2}^2\rangle$$

- DF/R [relativistic]: $Z\alpha \sim 0.25$ (Ge) / 0.4(Xe)
- RPA [random phase approximation]: residual $2e$ correlation induces configuration mixing in MB wave functions (including g.s.).

FCA vs. RPA: $\chi + A \rightarrow \chi + A^+ + e^-$



MB calculations need proper benchmark!

We tested our atomic methods against the database compiled by Henke et al.:
X-RAY INTERACTIONS: PHOTOABSORPTION, SCATTERING, TRANSMISSION, AND REFLECTION AT E = 50-30,000 eV, Z = 1-92
At. Data Nucl. Data Tables 54, 181 (1993).

Benchmark 1: S.P. Energies

Table 1

The single-particle energies of Ge atoms calculated by MCDF (s.p.) versus the edge energies extracted from photoabsorption data (edge) [29] of Ge solids. All energies are in units of eV.

	$K(1s_{\frac{1}{2}})$	$L_I(2s_{\frac{1}{2}})$	$L_{II}(2p_{\frac{1}{2}})$	$L_{III}(2p_{\frac{3}{2}})$	$M_I(3s_{\frac{1}{2}})$	$M_{II}(3p_{\frac{1}{2}})$	$M_{III}(3p_{\frac{3}{2}})$	$M_{IV}(3d_{\frac{3}{2}})$	$M_V(3d_{\frac{5}{2}})$	$N_I(4s_{\frac{1}{2}})$	$N_{II}(4p_{\frac{3}{2}})$	$N_{III}(4p_{\frac{1}{2}})$
s.p.	11185.5	1454.4	1287.9	1255.6	201.5	144.8	140.1	43.8	43.1	15.4	8.0	7.8
edge	11103.1	1414.6	1248.1	1217.0	180.1	124.9	120.8	29.9	29.3			

Table 1

The single-particle energies of a Xe atom calculated by DHF (s.p.) in this work versus the edge energies extracted from photoabsorption data (edge) in Ref. [18] (the one for the K-shell is not available). All energies are in units of eV.

	$K(1s_{\frac{1}{2}})$	$L_I(2s_{\frac{1}{2}})$	$L_{II}(2p_{\frac{3}{2}})$	$L_{III}(2p_{\frac{1}{2}})$	$M_I(3s_{\frac{1}{2}})$	$M_{II}(3p_{\frac{3}{2}})$	$M_{III}(3p_{\frac{1}{2}})$	$M_{IV}(3d_{\frac{5}{2}})$	$M_V(3d_{\frac{3}{2}})$
s.p.	34759.3	5509.8	5161.5	4835.6	1170.5	1024.8	961.2	708.1	694.9
edge	-	5452.8	5103.7	4782.2	1148.7	1002.1	940.6	689.0	676.4
	$N_I(4s_{\frac{1}{2}})$	$N_{II}(4p_{\frac{3}{2}})$	$N_{III}(4p_{\frac{1}{2}})$	$N_{IV}(4d_{\frac{5}{2}})$	$N_V(4d_{\frac{3}{2}})$	$O_I(5s_{\frac{1}{2}})$	$O_{II}(5p_{\frac{1}{2}})$	$O_{III}(5p_{\frac{3}{2}})$	
s.p.	229.4	175.6	162.8	73.8	71.7	27.5	13.4	12.0	
edge	213.2	146.7	145.5	69.5	67.5	23.3	13.4	12.1	

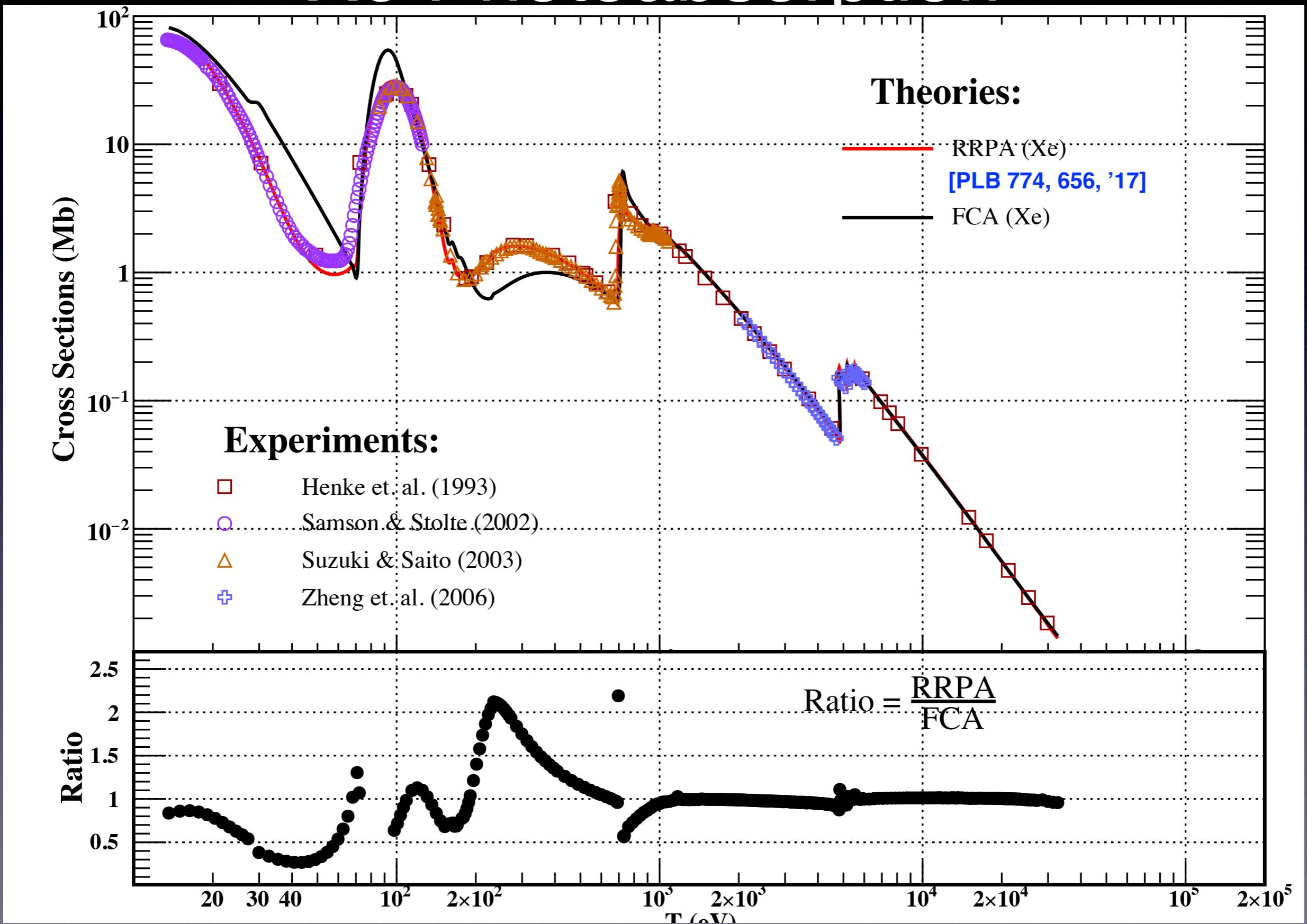
- Agreement is quite good for Xe and inner shells of Ge
- RHF agrees similarly, except no spin-orbit splitting
- Caution: this does not imply wave functions are good.

Benchmark 2: Photoabsorption

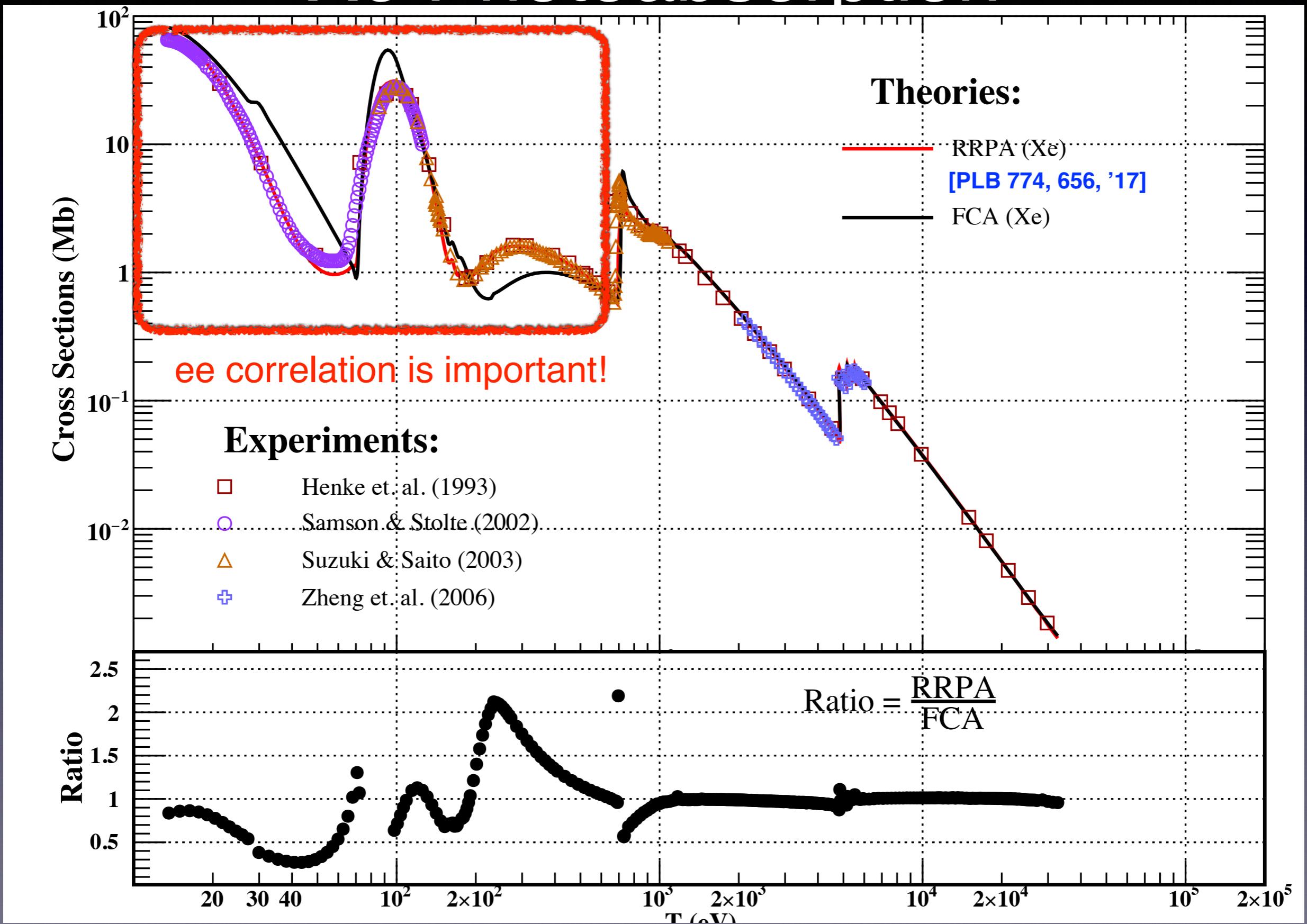


- Atoms respond by the transverse current $\vec{j}_\perp(\vec{q})$.
- Photon is **on-shell**, so $\mathcal{R}_{j_\perp}(T, q = T)$ can be determined by experiments.
- A true testing ground for the quality of the initial and final wave functions.

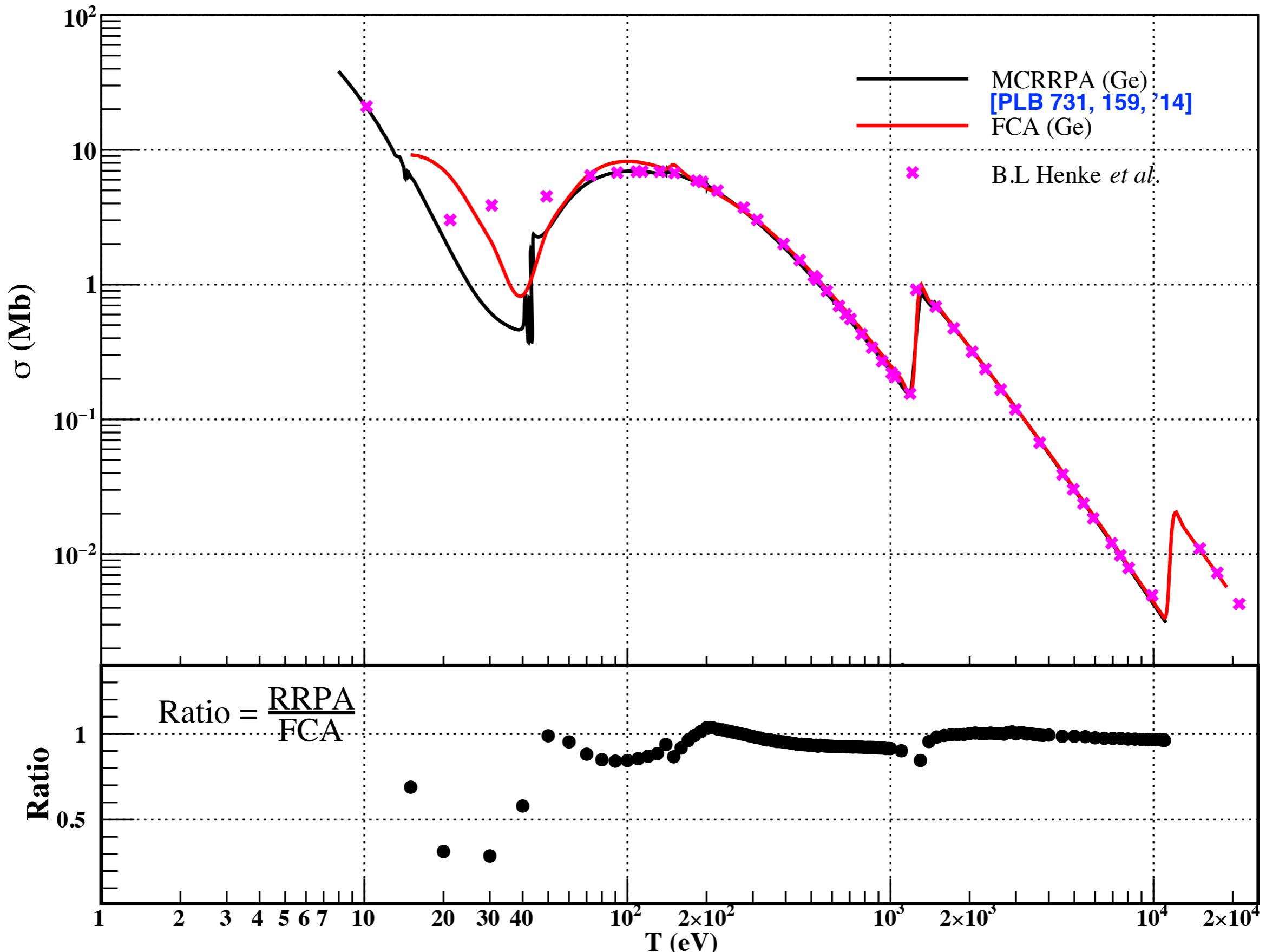
Xe Photoabsorption



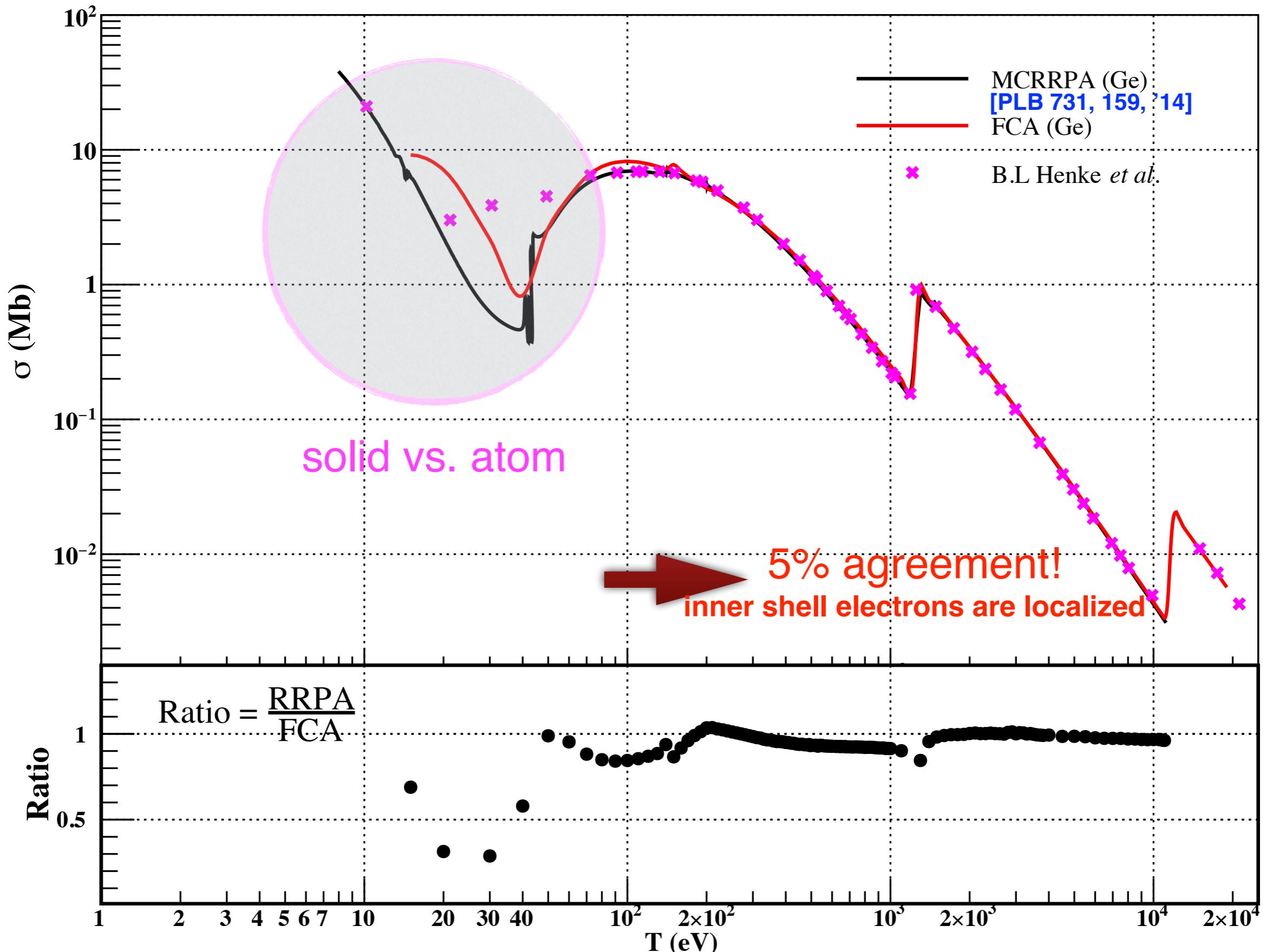
Xe Photoabsorption



Ge Photoabsorption



Ge Photoabsorption

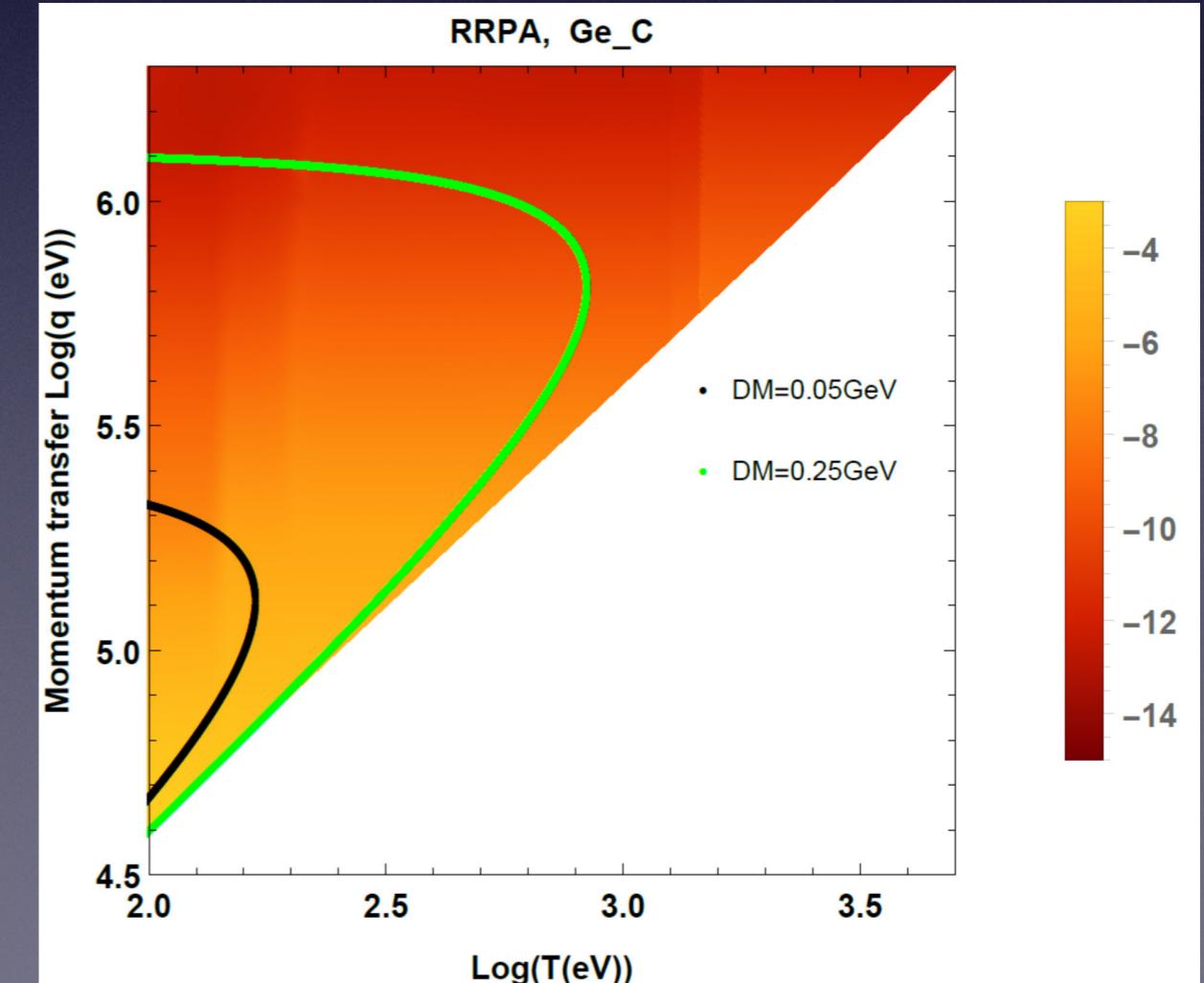
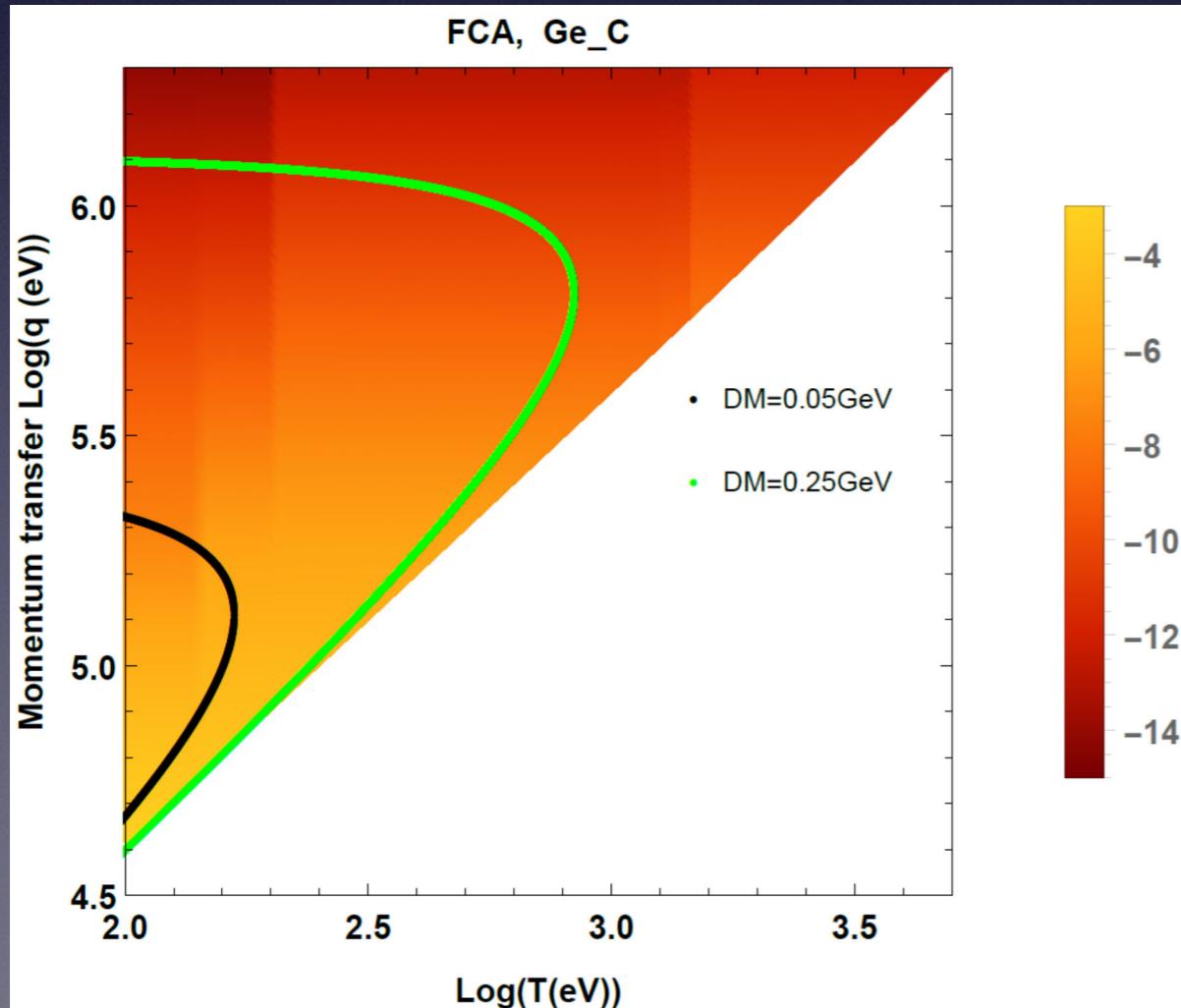


Progress & Outlook

- 1st version of the MCRRPA response functions for Xe and Ge ($T > 80\text{eV}$) with LO DM-electron interactions will be released after extensive testing (hopefully in a few months), along with the FCA ones and codes to compute dR/dT .

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Progress & Outlook

- Other atomic species (noble gas etc.), DM-electron interaction terms (NLO, NNLO), parameter space of (T, q) , other DM candidates (axions, ALPs etc.) [1] and neutrino BSM physics search [2] will be gradually added into the database.

[1] Wu, CPL et al., PRD 108, 043029 (2023) (inverse Primakoff effect; axio-electric effect is ongoing)

[2] Chen, ..., CPL et al., PRD 91, 013005 (2015); Hsieh, ..., CPL et al., PRD 100, 073001 (2019); ...

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STAY TUNED!