Global Searches and Optimisation in the Utilitarian Approach to Nuclear Excitation by Electron Capture (NEEC)

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Nuclear Excitation by Electron Capture (NEEC) involves the capture of an electron into a vacant atomic orbital, with the simultaneous excitation of the nucleus, assumed due to virtual photon exchange, and is a possible mechanism that can depopulate isomers in hot-dense astrophysical plasmas. The first observation of NEEC was reported in Nature 2018 [1], via the depletion of the 6.85hour 21/2⁺ isomer of ^{93}Mo in a beam-recoil-foil setup. The depletion probability was evaluated via a novel triple-coincidence gamma detection technique, with a resulting non-Coulomb excitation probability being attributed to the NEEC process with probability $P_{exc} = 0.01$. In a follow up paper [2], the theoretical calculation of the same scenario yielded an upper limit NEEC depletion probability of Pexc ≈ 10^{-11}. This depletion probability has been re-examined in [3], in which including the bound ^{nat}C target electrons allows a considerable increase and broadening in the collision and momentum density of available electrons. Thus the theoretical NEEC depletion probability has increased by up to an order of magnitude, the process being referred to as NEEC-Resonant-Transfer. Still it seems, there is an unknown mechanism at play to account for the remaining 8 orders of magnitude in unclaimed isomer depletion probability.

Currently one cannot ascertain the reason for this disparity without repeating the experiment under similar scenarios, and designing many NEEC and non-NEEC environments that can complement our understanding of the interaction space. This requires a holistic approach, including all possible types of experiment.

Theory <=> Experiment

Microscopic – S_{neec}

-If using the principle of detailed balance (PDB) neutral Internal Conversion Coefficients (ICC's) must be correctly scaled

The Microscopic Problem

$$\alpha_n = \left(\frac{|V_i|}{E_b^{q=0}}\right)^a \left(\frac{n_h}{n_{max}}\right)^b \alpha_{IC}^{q=0}$$

Scaling method modified from [4]

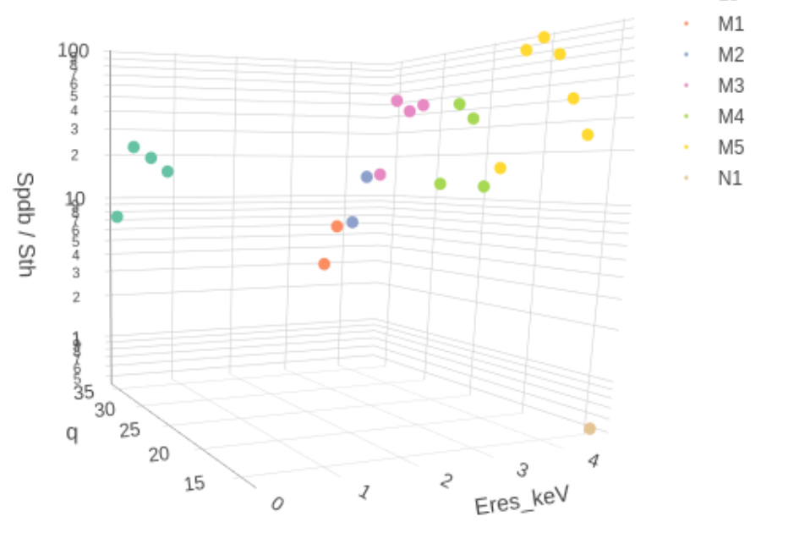


Figure 1: Overestimated scaling in ^{93m}Mo Ab Initio vs PDB Dataset; a=b=1

If a = -2 and b=2 then higher angular momentum subshells are more realistically scaled, see figure 4.

More *Ab Initio* Data Required to improve global estimates

"Malleable"
Rigorous with Temporal Limitations

Overlapping Microscopic with Macroscopic at Equilibrium

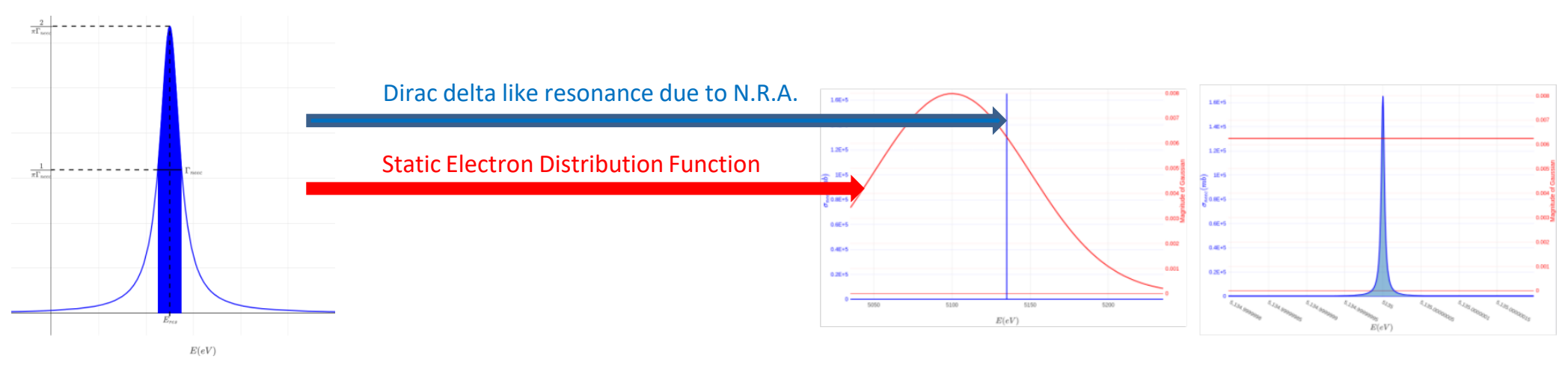
- Multiple instances of narrow resonance approximation (n.r.a.)

Microscopic

$$\sigma_{res}(E_e) = S_{neec}\frac{2}{\pi\Gamma_{neec}}$$

Macroscopic

$$\boldsymbol{\phi_e} = n_{i-e}(t)v_eF(E_e)$$



$$S = \frac{2\pi^2}{p^2}\frac{A_r^{d\to f}}{\Gamma_d}Y_{neec}^{i\to d}$$

$$Y_{neec}^{i\to d} = \frac{(2J_d+1)(2j_{at}+1)}{2(2J_i+1)}\alpha_n^{d\to i}A_r^{d\to i}$$

$$R_{neec} = n_{i-e}v_{res}\sigma_{res}\int_{E_{res}-\frac{\Gamma}{2}}^{E_{res}+\frac{\Gamma}{2}} F(E)dE$$

$$R_{NEEC} = \Sigma_{q,\alpha}P_qR_{neec}^{q,\alpha}$$

$$N_{neec} = R_{NEEC}\,\tau_p^{tot}$$

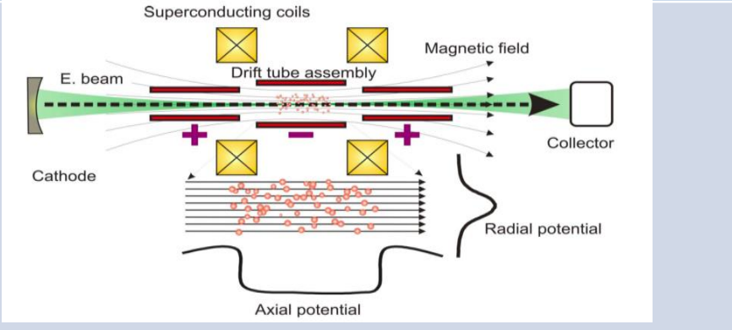
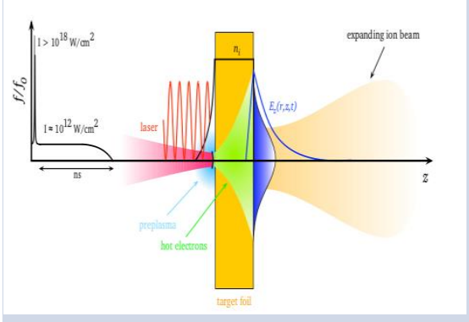
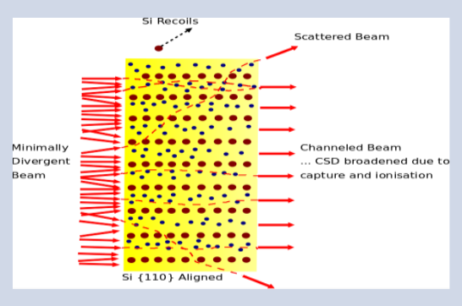
A proper Candidate Search should be:

1. Malleable
2. Rigorous
3. Complete

Macroscopic – R_{neec}

- Must have a realistic and computable continuum distribution function partitioning a chosen limit on the ion-electron density

Ion-Electron Density – n_{i-e}[cm^{-3}]: $n_{i-e} = \int_{V_{int}} n_{elec}n_{ion}dV$

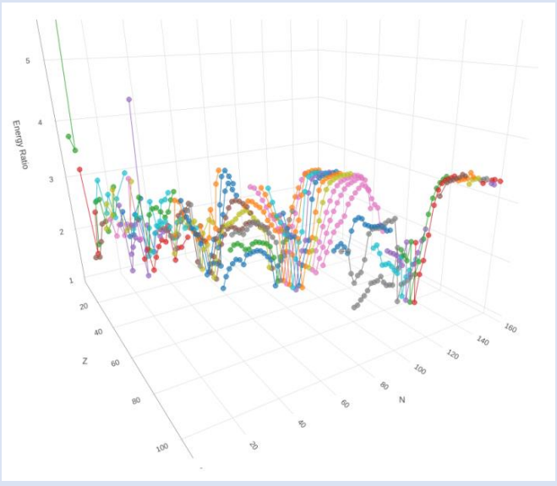
Approach	Electron Beam Ion Trap	Plasma	Beam-Foil
Diagram	 [2]	 [2]	
e^- Number Density (cm^{-3})	n_e < 1E12	n_e < 1E24	n_e < 1E23
Ion Number Density (cm^{-3})	n_{ion} < 1E10	n_{ion} < 1E10	n_{ion} < 1E10
Interaction Volume (cm^3)	V_{int} < 1E-4	V_{int} < 1E-5	V_{int} < 1E-2
Ion-Electron Density	n_{i-e} < 1E18	n_{i-e} < 1E29	n_{i-e} < 1E31
Comment:	Can Polarise the Electron Beam Increases resonance strength by ~2 orders of magnitude		Channeled Fraction < 1E-4 n_{i-e} < 1E27 Can increase this by an order of magnitude by considering bound target electrons

"Malleable"
Rigorous

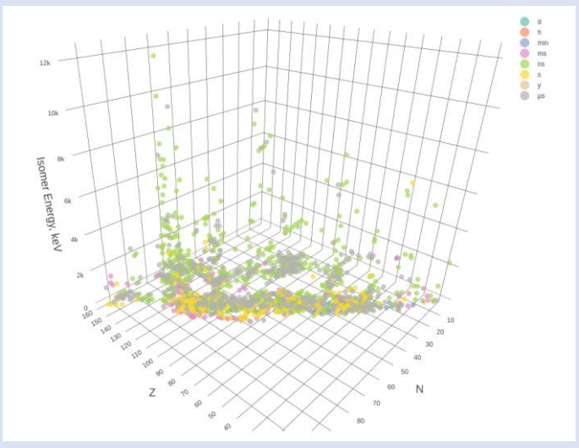
NEEC Candidate Database

Currently one cannot ascertain the reason for the experimental NEEC disparity without repeating the experiment under similar scenarios, and designing many NEEC and non-NEEC environments that can complement our understanding of the interaction space. This requires a holistic approach, including all possible types of experiment.

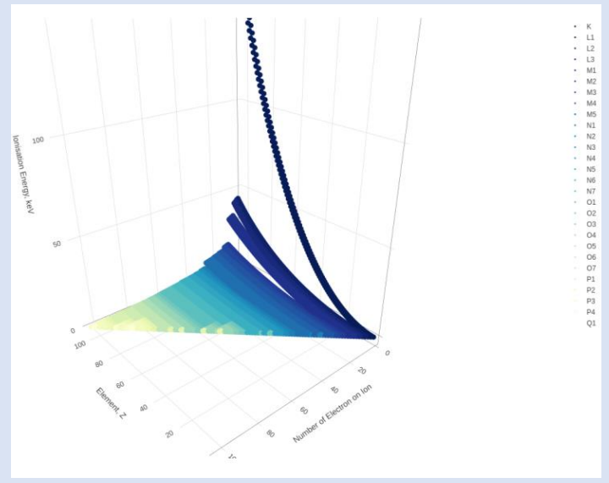
- ENSDF (NNDC) data is parsed from the archaic raw database

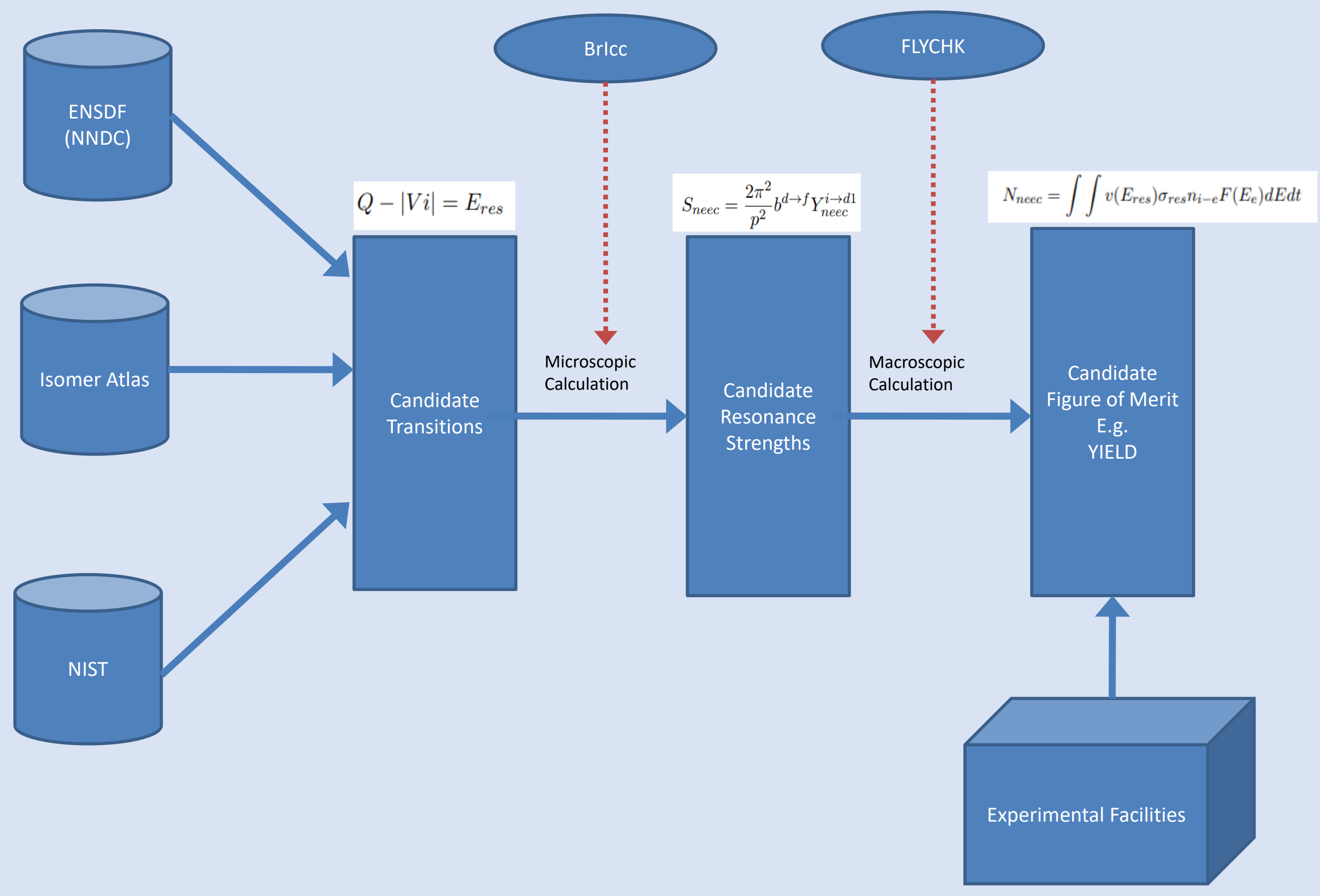


- The Atlas of Nuclear Isomers is used as a database of metastable nuclear states and is a more complete list of nuclear isomers than ENSDF.



- The NIST Database provides all atomic ionisation energies which are equivalent to electron binding energies for ground state atomic shells from within a non-IPD continuum.





ENSDF (NNDC)

Isomer Atlas

NIST

BrIcc

FLYCHK

$Q - |Vi| = E_{res}$

Candidate Transitions

Microscopic Calculation

$S_{neec} = \frac{2\pi^2}{p^2}b^{d\to f}Y_{neec}^{i\to d1}$

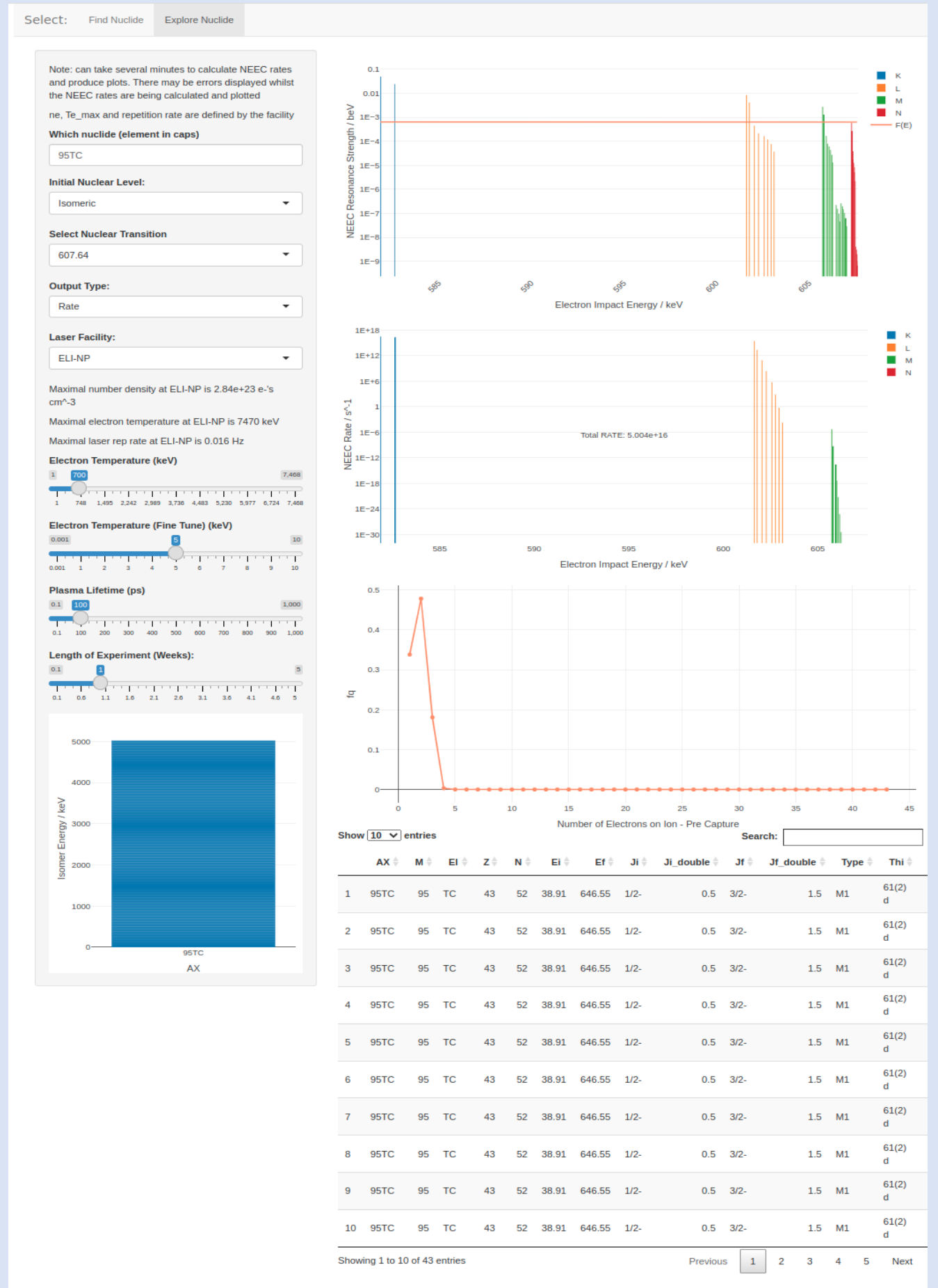
Candidate Resonance Strengths

Macroscopic Calculation

$N_{neec} = \int\int v(E_{res})\sigma_{res}n_{i-e}F(E_e)dEdt$

Candidate Figure of Merit E.g. YIELD

Experimental Facilities



Showing 1 to 10 of 43 entries

Previous 1 2 3 4 5 Next

Figure 2: The relational database requires a user interface
All NEEC candidates that exist are within and are optimisable via the user interface

"Complete"

"Complete"

Results of the Database – Promising Isomers and Astrophysical Use

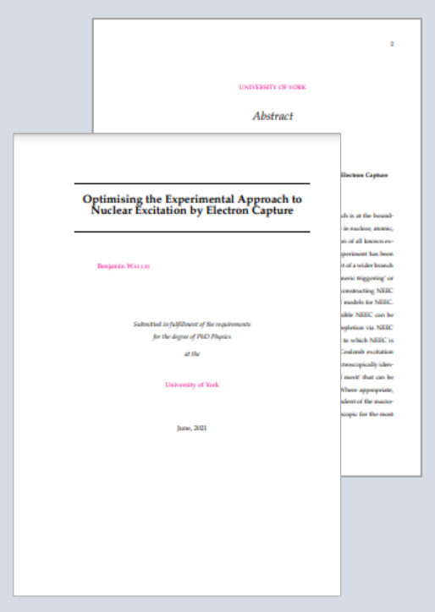
To assist in design and enhance the extent to which theory and experiment can be compared, we have developed a systematic NEEC tool, which combines via modern data-science techniques the NIST and ENSDF databases along with the BrIcc and FLYCHK companion tools. This allows the experimenter to choose an appropriate initial species and optimise macroscopic parameters in the chosen experimental approach, with a microscopic scaling allowing NEEC resonance strengths to be accurate to within an order of magnitude or better. Concurrently, we can express how such a tool can be used to evaluate the astrophysical impact of NEEC across the entire nuclear chart.

~20,000 transitions total

Plasma… top 10… unknown Reduced Transition Probability

AX	Ei (keV)	Ef (keV)	Ji	Jf	Type	$T_{1/2}$ initial	$T_{1/2}$ final	Occ	CS	Config	subshell	J_{atomic}	|Vi| (keV)	|Vi| mean (keV)	Q (keV)	E_e keV	E_{ion} MeV/u	B (w.u.)	Ar (s^{-1})	$\Gamma_{t1/2}$ (eV)	$\Gamma_{Ar(1+\alpha)}$ eV	α_k	α_{tot}	S_k beV	S_{tot} beV	Rate Plasma α_{tot} Ion^{-1} s^{-1}	Rate EBIT s^{-1}
165YB	126.8	132.5	9/2+	7/2+	M1	300(30) ns	2.8 NS	15	55	3p3	M3	1.5	5.34	5.46	5.69	0.351	0.64	1	5866320.389	1.63E-07	7.70E-08	18.947	591	2.51	156.84	1.63E+08	1.22E-01
238U	2,557.9	2,593.7	0+	1-	E1	280(6) ns	4.1E-3 EV	3	89	2s	L1	0.5	32.84	8.28	35.80	2.9635	5.44	1	1.80261E+11	0.002841903	0.000180261	0.519	1.87	467.61	464.01	4.22E+07	6.57E+01
235U	0.1	13.0	1/2+	3/2+	M1	~ 26 min	0.50 NS	11	81	3s	M1	0.5	12.16	8.28	12.90	0.7385	1.36	1	68335535.66	9.13E-07	3.06E-05	679.207	476	621.84	181.75	4.16E+07	4.37E+01
238U	2,557.9	2,602.5	0+	1-	E1	280(6) ns	1.9E-3 EV	3	89	2s	L1	0.5	32.84	8.28	44.60	11.7635	21.60	1	3.48543E+11	0.00131698	0.00030942	0.349	1.047	151.65	377.47	2.95E+07	4.19E+01
152EU	77.3	89.8	3-	4+	E1	38(4) ns	384 NS	14	49	3p2	M2	1.5	4.40	4.68	12.59	8.1903	15.04	1	5814841155	1.19E-09	6.73E-06	0.758	14.73	6.80	166.08	2.89E+07	1.58E+00
82Y	507.5	511.8	6+	5-	E1	147(7) ns	1.42 NS	27	12	3p63d9	M5	2.5	0.41	2.36	4.32	3.906	7.17	1	155666216.5	3.21E-07	2.34E-07	1.288	107.6	0.64	72.37	2.55E+07	1.03E-01
219RN	4.5	14.4	9/2+	7/2+	M1	15.4(13) ns	875 PS	13	73	3p	M2	1.5	9.78	7.45	9.90	0.12	0.22	1	30898298.39	5.21E-07	2.17E-06	105.577	564	215.31	73.00	2.31E+07	6.11E+00
163YB	124.0	132.5	9/2+	7/2-	E1	~ 10 ns	1.15 NS	14	56	3p2	M2	1.5	5.73	5.46	8.50	2.769	5.08	1	1874630771	3.97E-07	4.10E-06	2.320	11.88	12.41	74.89	2.12E+07	1.69E+00
161DY	25.7	43.8	5/2-	7/2+	E1	29.1(3) ns	0.99 NS	3	63	2s	L1	0.5	15.23	5.01	18.15	2.92658	5.37	1	18115378098	4.61E-07	3.81E-05	2.196	5.93	89.47	133.14	1.79E+07	1.25E+01
172LU	41.9	109.9	1-	2+	E1	3.7(5) min	2.30 NS	3	68	2s	L1	0.5	17.93	5.58	67.99	50.06195	91.92	1	9.94385E+11	1.98E-07	0.000737503	0.127	0.945	19.79	300.14	1.73E+07	1.07E+01

To ensure the future validity of this search tool we include all unknown-strength electromagnetic transitions and use Weisskopf estimates. This allows the parameter space to be model independent globally until a model can be applied in the chosen nuclear transition optimisation.



See Thesis
For rigorous optimisation parameter-space

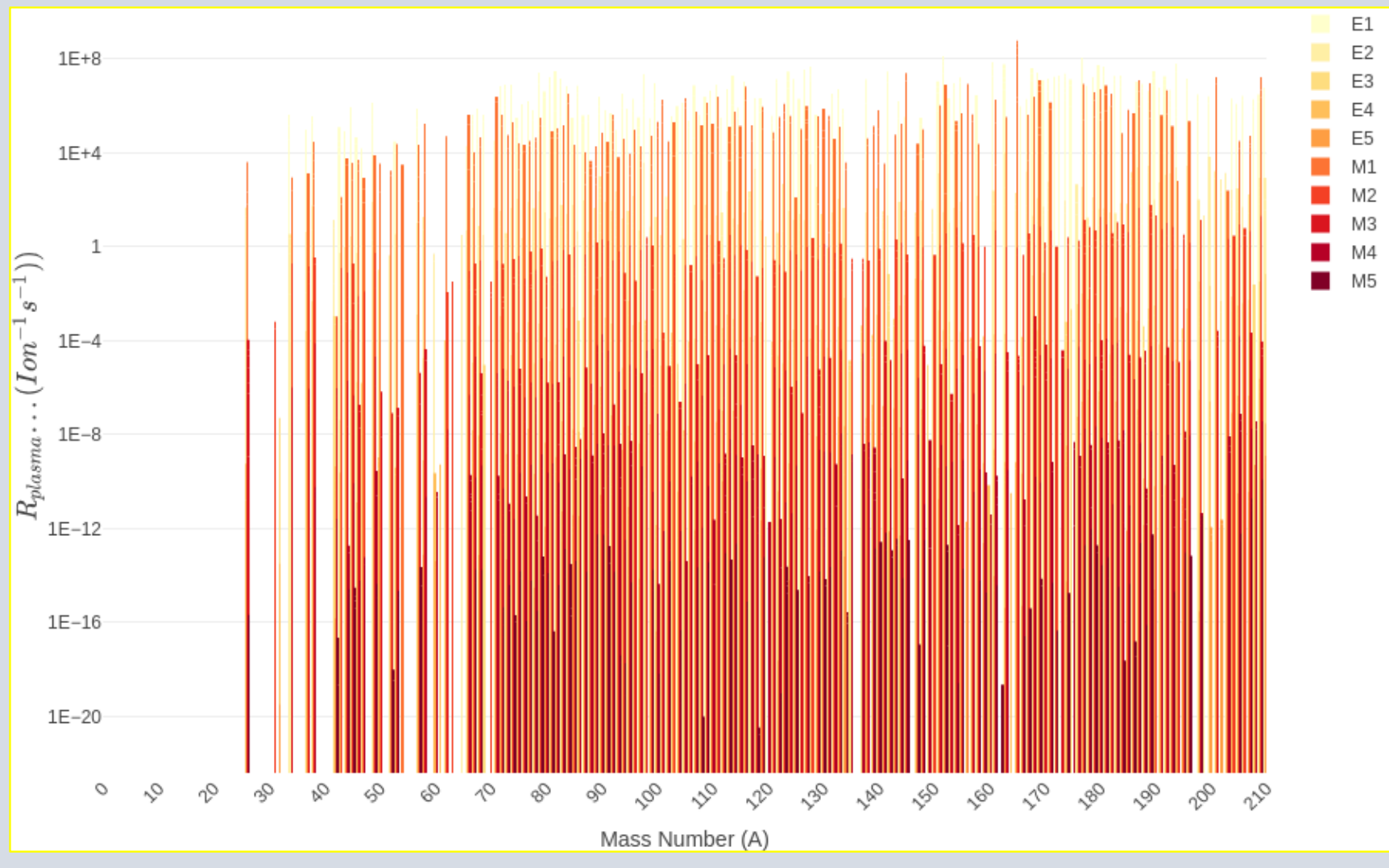


Figure 3: Isomeric depletion transitions that are possible within a terrestrial plasma. The rate is per ion. A large increase in the size of the parameter space is involved with inclusion of all laser-plasma parameters and ion influx techniques, but still can be rigorous

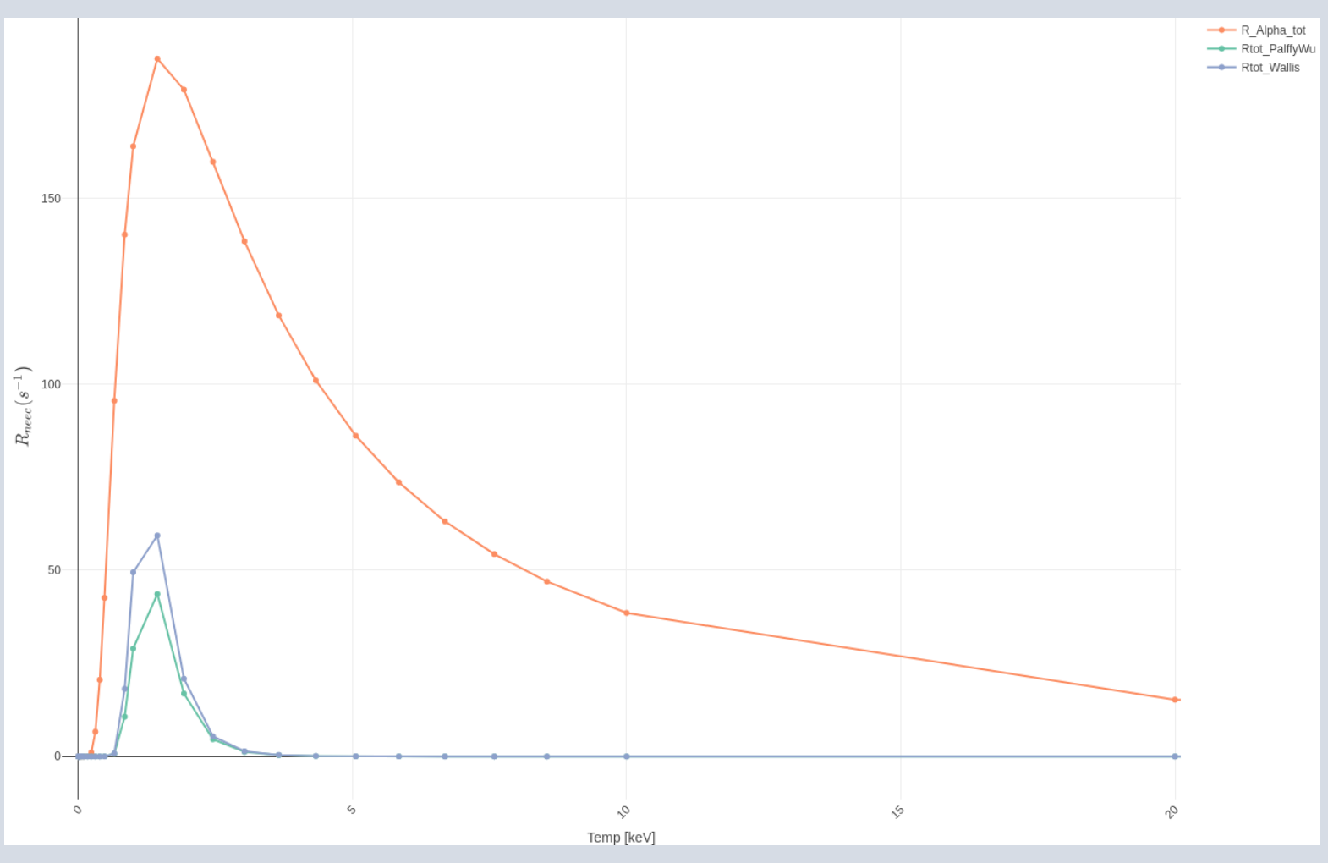


Figure 4a: Optimal Temperature for ^{93}Mo optically generated plasma with n_e = 1E24 cm^{-3}

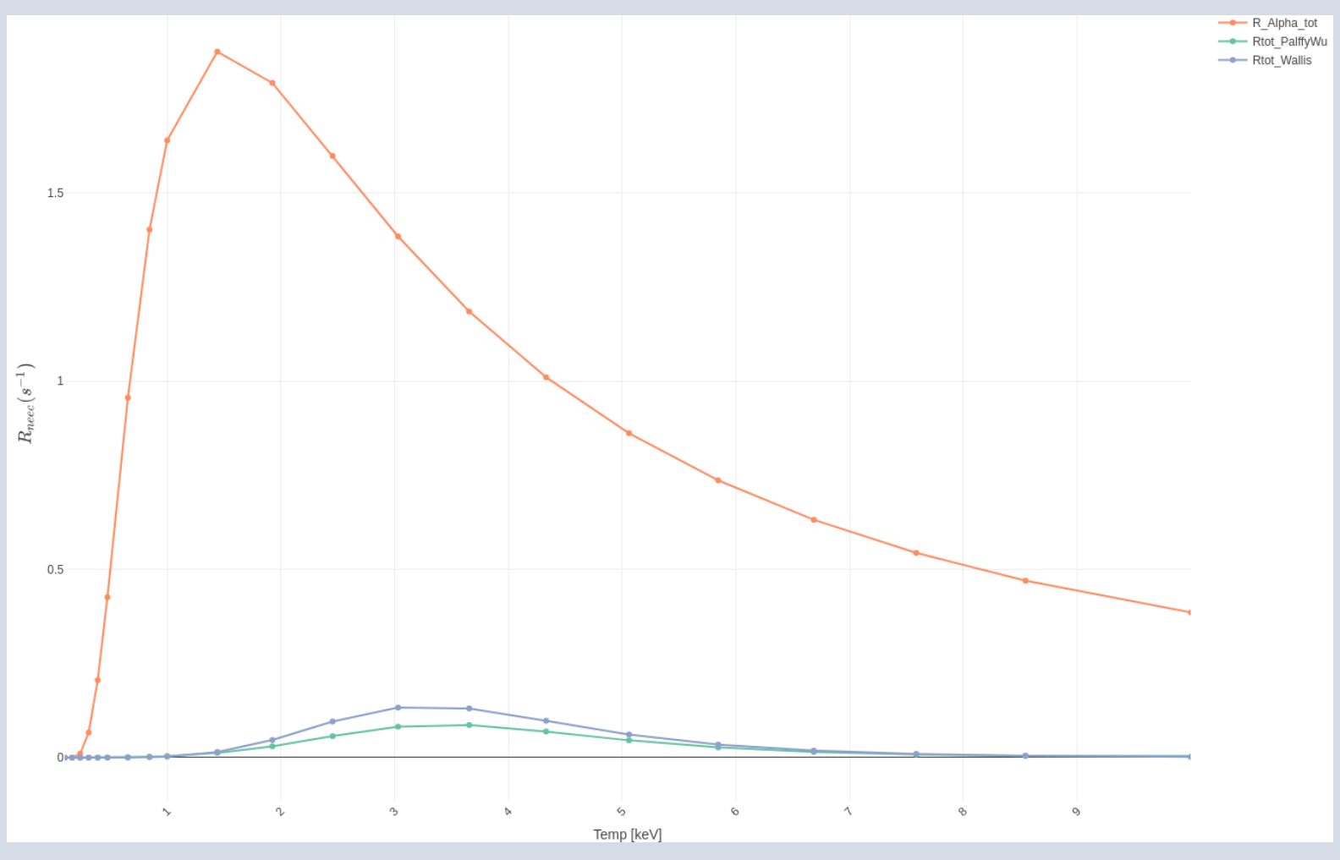


Figure 4b: Optimal Temperature for ^{93}Mo optically generated plasma with n_e = 1E22 cm^{-3}

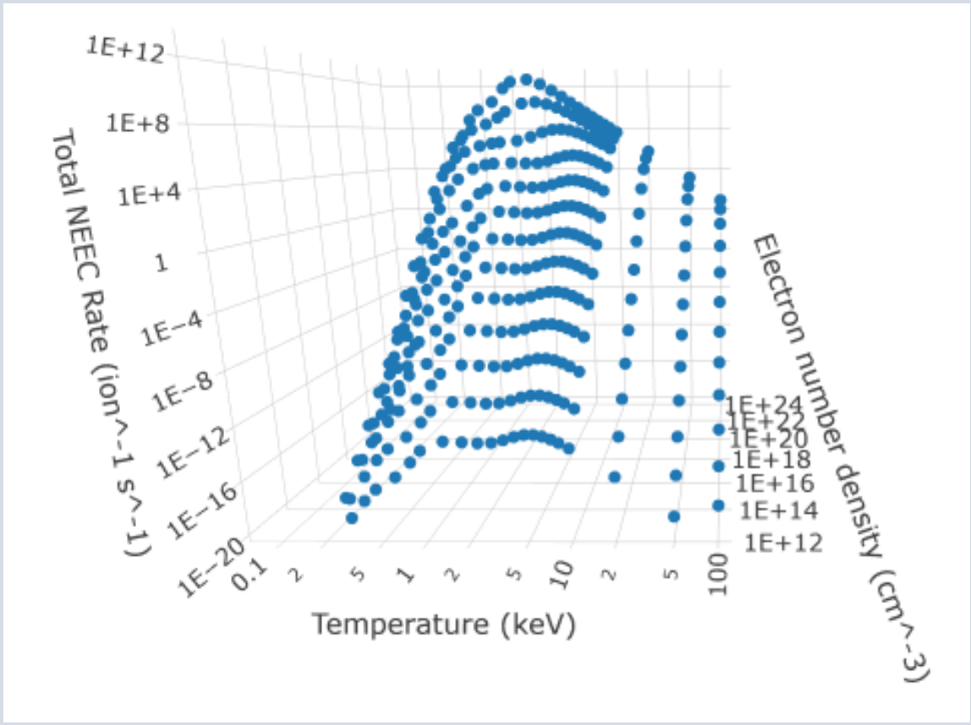


Figure 4c: Surface for finding the optimal {T_e,n_e} NEEC environment for ^{93m}Mo. This can be produced for any of the ~20,000 candidate NEEC transitions within FLYCHK temperature ranges

In figure 4 calculations are compared to method via [5] for optical laser generated plasma. It is evident that using α_{tot} and mean impact energies it is reasonable to estimate with better than an order of magnitude in the NEEC rate, but without knowledge of where the optimum lies. One can locate the optimal temperatures with the scaling a=b=1 suggested in [4], but with very large over-scaling of the NEEC rate into high angular momentum subshells. The accuracy in the rates can be within 20% of *Ab Initio* if using a=-2, b=2.

Overarching Conclusion

- **Internal Conversion Coefficients can be scaled to produce considerably accurate (within 20%) NEEC rates in n-LTE plasma using scaling constants a=-2 and b=2.**
- **The NEEC Database is accessible, malleable, complete, and rigorous, allowing NEEC experimental design to be conversive with theory**
- **As a result, the astrophysical implications of NEEC depletion can be analysed globally**

[1] C. J. Chiara et al. "Isomer depletion as experimental evidence of nuclear excitation by electron capture". Nature Publishing Group 554.7691 (2018),pp.216–218.issn:0028-0836. doi:10.1038/nature25483.url:http://dx.doi.org/10.1038/nature25483.
[2] Y. Wu, C. H. Keitel, and A.Pálffy. "93mMo isomer depletion via beam-based nuclear excitation by electron capture". physical review letters(mar. 2019). doi: 10.1103/physrevlett.122.212501. url: http://arxiv.org/abs/1904.00809. url: http://dx.doi.org/10.1103/physrevlett.122.212501.
[3] J. Rzadkiewicz et al. "Novel approach to Mo93m isomer depletion: nuclear excitation by electron capture in resonant transfer process". in: physical review letters 127.4 (july 2021), p.042501. issn: 0031-9007. doi: 10.1103/physrevlett.127.042501. url: https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.127.042501.
[4] S.Gargiulo, I. Madan, and F.Carbone. "Nuclear Excitation by Electron Capture in Excited Ions". In: Nuclear Theory (Feb. 2021). URL: http://arxiv.org/abs/2102.05718.
[5] Jonas Gunst et al. "Nuclear excitation by electron capture in optical-laser-generated plasmas". In: Plasma Physics (2018), pp. 1–18