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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 $P_{exc} \sim 10^{-11}$. 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.

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.

[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.

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