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Electronic Structure of Superheavy Elements 116 and 117

Garry Vong, Victor Flambaum, Vladimir Dzuba

School of Physics, University of New South Wales, Sydney 2052, Australia

INTRODUCTION & MOTIVATION

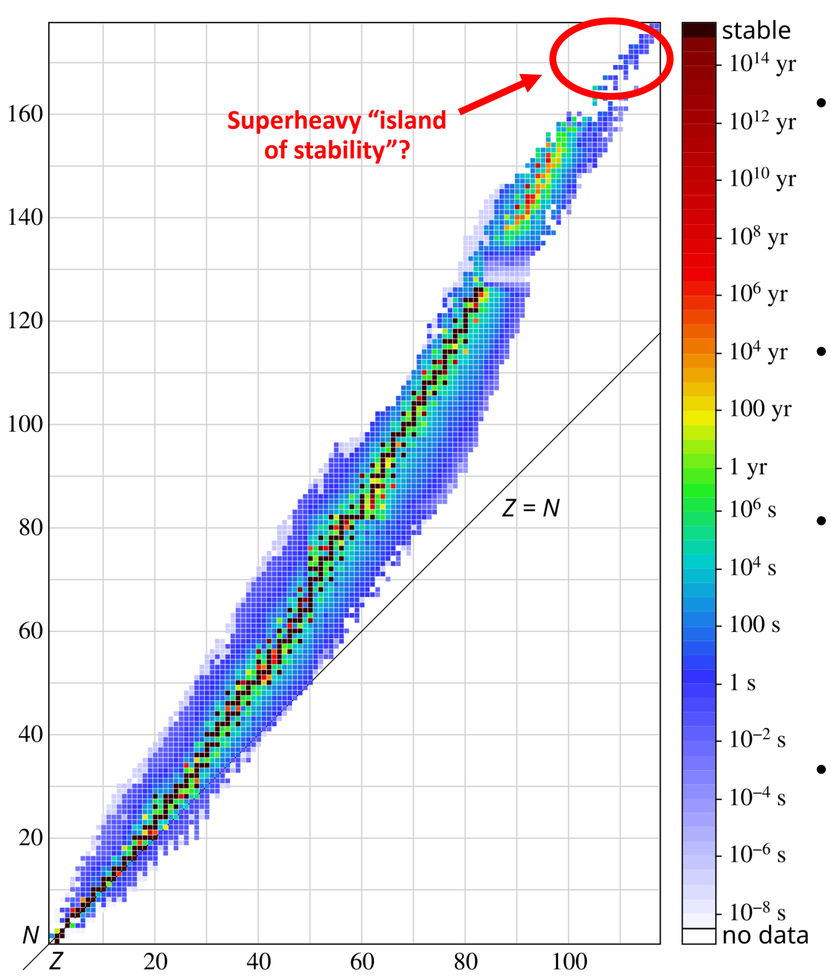

Figure 1: Chart of half-life of known isotopes. Predicted island of stability is circled.

- **Scarcity of experimental and theoretical data** on spectroscopy of superheavy elements (Z > 102).
- **Search for the "island of stability"**, where longer-lived isotopes may exist.
- **Stringent test of computational methods** under extreme relativistic and strong correlation effects.
- **Low energy probe for new physics**, alternative to high energy searches.

METHOD

Dirac Hartree-Fock Method

Mean field potential is calculated for the closed core (by removing M electrons):

$$\hat{H}^{\mathrm{RHF}} = c\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + (\beta - 1)mc^2 + \mathrm{V}_{\mathrm{nuc}} + \mathrm{V}^{N-M}$$

Coupled-Cluster Single-Double Method

Single and double electron correlation effects from core to valence states are computed:

$$\hat{\Sigma}_1, \hat{\Sigma}_2$$

Configuration Interaction with Perturbation Theory

States are calculated using the mean field potential and electron correlations:

$$\hat{H}^{\mathrm{CI}} = \sum_i^M \left(\hat{H}^{\mathrm{RHF}} + \hat{\Sigma}_1\right)_i + \sum_{i<j}^M \left(\frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} + \hat{\Sigma}_{2ij}\right)$$

Compare with Experimental Data

The accuracy of calculations is benchmarked against lighter elements with similar electronic structure.

RESULTS

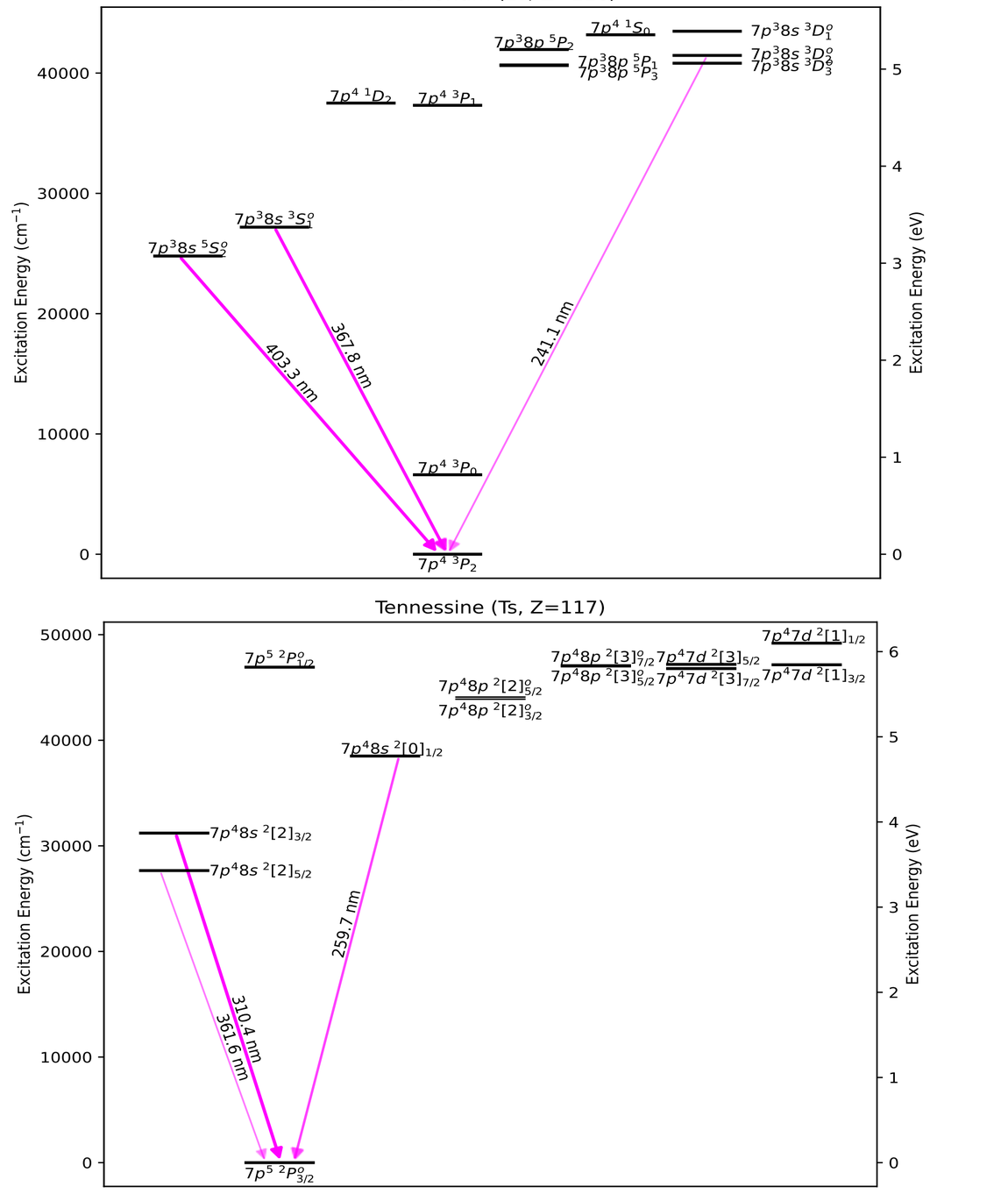

Figure 2: Calculated excitation energies of **a) l**ivermorium and **b)** tennessine. Optical electric dipole (E1) transitions that are predicted to have strong transition amplitudes are also shown.

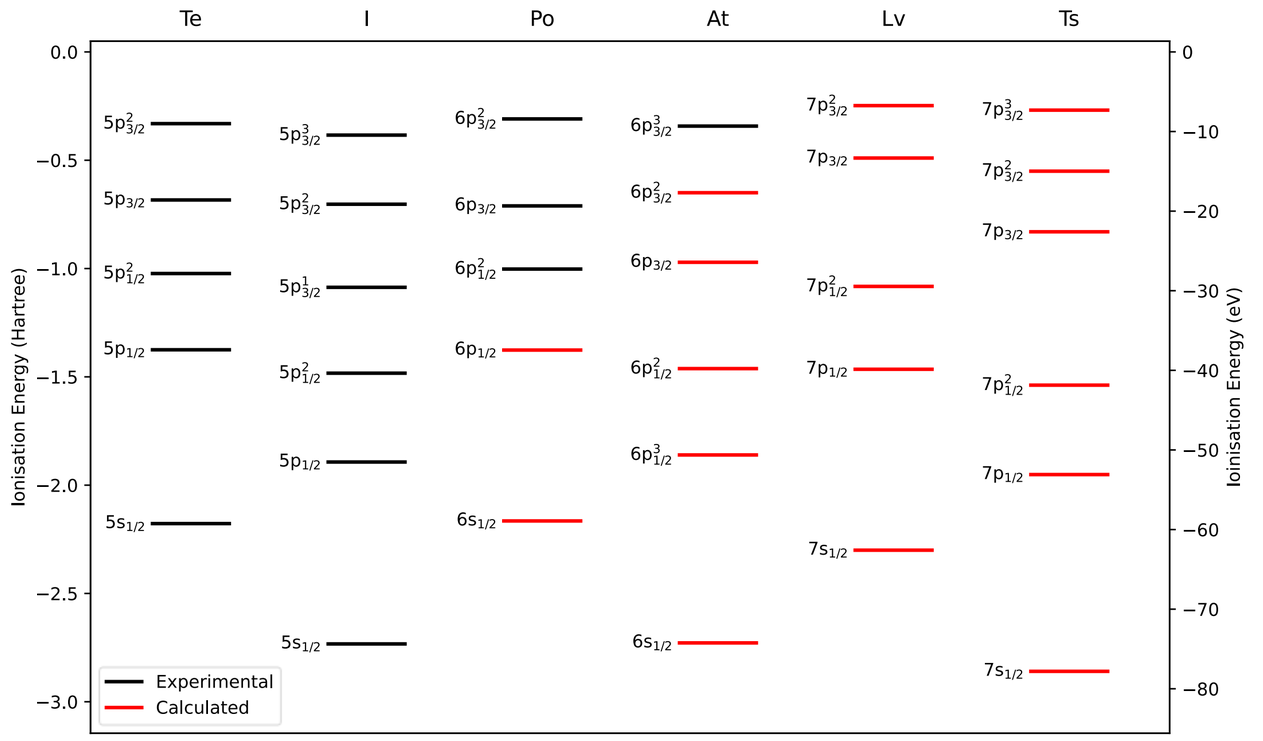

Figure 3: Experimental and calculated ionisation energies are presented for livermorium and tennessine along with their lighter homologues.

CONCLUSION

- Fills critical gaps in spectroscopic data for superheavy elements.
- Demonstrates the viability of this approach for many-body calculations with extreme relativistic effects and strong electron correlations.
- Provides theoretical benchmarks for future experiments.

REFERENCES

[1] V. A. Dzuba, V. V. Flambaum, and G. K. Vong, Physical Review A 112, 012822 (2025)
[2] G.K. Vong, V.A. Dzuba, and V.V. Flambaum, Atomic Data and Nuclear Data Tables, 101769, 0092-640X (2025)