High-performance atomic structure calculations and the search for new physics

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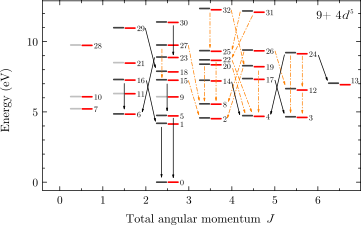
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**Précis: We present new extensions and techniques in atomic structure calculations, with a focus on applications to the search for physics beyond the standard model.**

Recent improvements in experimental spectroscopy of highly-charged ions and superheavy atoms have enabled a range of new applications in fundamental and applied physics, such as low-energy tests for physics beyond the standard model[1], high precision metrology [2], and EUV photolithography [3]. These applications require systems with open-shell electronic structures and strong many-body correlation effects, which present considerable challenges to accurately model.

One computational approach which has produced promising results for open-shell atoms and ions is Configuration Interaction with Many-Body Perturbation Theory (CI+MBPT). This technique has been used to accurately predict the structure of atoms and ions with up to four valence electrons [4,5], but is known to suffer from severe limitations for larger numbers of electrons.

We will present recent results from our high-performance atomic structure code AMBiT - a modified CI+MBPT implementation which employs the particle-hole formalism to treat open-shell systems with high accuracy. Recent calculations have shown that AMBiT is capable of predicting the optical spectra of highly-charged tin ions with open d-shell configurations with less than 1% error [3]. AMBiT employs a number of new theoretical and computational techniques to achieve this level of accuracy; including the particle-hole formalism and extensive modifications to CI and MBPT. We will provide a detailed overview of these modifications and highlight AMBiT's advantages compared to existing atomic structure codes. These results represent the cutting-edge of atomic structure calculations for many-valence electron systems and provide a benchmark for next-generation precision tests.



*Comparison of experimentally determined optical spectra of Sn9+ ions (grey) against spectra calculated by the AMBiT atomic structure code (red). Energy levels shown are the fine-structure splitting of the 4d5 configuration ground state. Adapted from [3]*

**References**

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