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## Calculations with parametric CI-MBPT method of properties of complex atoms

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Many complex atoms, such as actinides, present difficulties for theory. The difficulties are manifold: 1) valence electrons interact strongly, requiring generation and eigen solution of a large matrix to treat the interaction accurately; 2) many valence electrons interact strongly with 86 core electrons, and these interactions have to be taken into account beyond the small-perturbation level; 3) relativistic effects are very important, affecting the order of closely spaced levels and many atomic properties. Currently there are no calculations demonstrating accurate energy levels and other properties of the neutral U atom or other actinides. The only method that has been used throughout the world so far is a multi-configuration Hartree-Fock (MCHF) approach, developed by Cowan at LANL more than 30 years ago, and which contains various fitting parameters. Configuration-interaction many-body perturbation theory (CI-MBPT) is a promising method, since it demonstrated high accuracy in light multi-valence atoms. However, valence-core interactions in actinides are very strong to be treated in the second-order MBPT, used in the CI-MBPT method. One solution is the CI-All-order method, but it is quite time consuming and rather complex. An alternative solution is to introduce fitting parameters into CI-MBPT to account for valence-core, relativistic and omitted valence-valence interactions. Using this parametric CI-MBPT approach it is possible to match energy levels with the precision of about 100 inverse cm for atoms such as Th and U III. This resulted in simplification of matching theoretical and experimental levels, and quite accurate g-factors. Some preliminary calculations have also showed that the theory can predict oscillator strengths. Examples of Xe I, Y I, U I, Th I and other atom calculations will be given to demonstrate improved accuracy of the CI-MBPT approach. This is just first attempts showing great promise of the parametric CI-MBPT approach to actinide atoms.

### Biography

Igor M Savukov has completed his PhD in 2002 at the University of Notre Dame, IN USA, and in 2006 his postdoctoral studies at Princeton University. Currently, he is an R&D Scientist at Los Alamos National Laboratory. He has published 80 papers in reputed journals, h index 22, and has been working over 20 years in the field of atomic structure calculations especially in the field of relativistic many-body theory.

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