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Applications of many-body perturbation theory to actinide atoms

There are three main challenges for accurate applications of atomic theory to calculations of energy levels and other properties of Actinide atoms. First, the valence-valence interaction is strong and requires a large configuration space to account for this interaction. Various methods have implemented small configuration space and cannot account for the interaction with highly excited states and continuum. Second, the valence-core interaction is also strong and second-order MBPT, which is usually implemented in the configuration-interaction (CI) many-body perturbation theory (MBPT) method, is not adequate. Finally, the relativistic effects are significant breaking the LS-coupling scheme and making the transition amplitudes sensitive to these corrections. The approach of relativistic CI-MBPT is quite promising. It proved to give quite accurate results in light atoms, where the valence-core interaction can be described well in the second order and relativistic effects can be accounted for by employing Dirac-Fock basis and adding dominant Breit interactions. However, ab *initio* CI-MBPT completely fails in actinides. Still, significant improvement in accuracy can be achieved by introducing adjustable parameters. In particular, seven such parameters can be used to correct the single-valence energy, while additional two parameters can be used to improve the Coulomb screening. With 9-parameter CI-MBPT approach it is possible to reproduce energy levels in as complex an atom as U I. In this talk, I will show examples of CI-MBPT calculations with adjustable parameters for complex atoms. The work is in progress and some future directions will be also discussed.

Biography

Igor M Savukov has completed his PhD in 2002 at the University of Notre Dame, in the 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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