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Ab *initio* precision CI-MBPT calculations for noble-gas atoms

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Noble gas atoms, important for plasma modeling and other applications are quite difficult for theoretical calculations because of large correlation and relativistic corrections. In particular, the particle-hole configuration-interaction many-body theory (CI-MBPT) has difficulties due to poor convergence of MBPT for the "hole" states. Recently we found that MBPT convergence and the accuracy of CI-MBPT can be improved by treating eight hole upper s- and p- electrons as valence electrons and by restricting the number of configurations in a certain way to make computation time manageable. We analyzed a large number of transition in Ar and other noble-gas atoms and found that Ar and Ne calculations are in good agreement with experiment, while calculations in heavier noble-gas atoms agree less with experiments, which partially can be attributed to the experiments. Because transition probability data are limited, we also analyzed intensities of discharge emissions, which at certain conditions are correlated with experimental transition probabilities and found that such correlation exists with theoretical calculations as well, especially in the cases where detection efficiency has been carefully taken into account.

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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