

Abstract Submitted
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CI-MBPT energy levels of four-valent Si I IGOR SAVUKOV, Los Alamos National Laboratory — The mixed configuration-interaction many-body perturbation theory (CI-MBPT) method is accurate in divalent atoms. In more complex atoms, with the number of valence electrons it becomes progressively more difficult to saturate CI space. Here a four-valence electron atom, Si I, is considered. It is found that by using a relatively small cavity of 30 a.u. and by choosing carefully configuration space, it is possible to obtain quite accurate agreement between the theory and experiment. After subtraction of systematic shifts of 481 cm^{-1} and -426 cm^{-1} for the lowest even states and odd states respectively, the deviation between theory and experiment becomes at the level of 100 cm^{-1} . This agreement is comparable to that in divalent atoms where the CI saturation has been achieved. It is anticipated that the approach can also give good results for atoms with more valence electrons to be considered in the future.

Igor Savukov
Los Alamos National Laboratory

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