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Relativistic configuration interaction with core polarization method for the divalent systems

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Synopsis   The relativistic configuration interaction with core polarization method and program for the divalent systems have been developed. Based on this new program, the energy levels, transition matrix elements, static and dynamic dipole polarizabilities of He, Be, and Mg atoms have been calculated systematically.

The divalent atoms have been widely used in high-precision physics, such as, atomic clock, quantum information. The divalent systems are of the advantageous candidates in atomic clocks because its narrow spin-forbidden transition is less susceptible to effect of the external field. The main uncertainties of these high-precision measurements are from the blackbody radiation shifts and ac stark shifts. The static and dynamic polarizabilities of the divalent atoms are very important to evaluate these uncertainties.

The relativistic semiempirical core polarization method has already succeeded in computing the atomic structures of monovalent systems previously [1]. Recently, the relativistic configuration interaction with core polarization(RCICP) method has been developed by us to deal with the divalent systems. The basic strategy is in a frozen core model in which the atoms are partitioned into valence and core electrons. The wave functions of core electrons are represented by the Dirac-Fock calculations. The single electron orbitals are expanded in a large basis of L-spinors and S-spinors, which can be regarded as relativistic generalizations of the familiar Laguerre- and Slater-type orbitals respectively. The total number single electron orbitals usually can be extended to 1000 in the present program. The wave functions of atomic states are built as a linear combination of two valence electron configurations of the same J-value and parity. Core-valence correlations are represented by introducing semiempirical one- and two-body core polarization potentials, which are tuned to ensure that the energies for the valence electrons agree with experiments.

Table 1. The static dipole polarizabilities (in a.u.) of the ground states of He, Be, and Mg atoms.

Method	He $1s^2$	Be $2s^2$	Mg $3s^2$
RCICP	1.38306	37.61	70.32
CICP [2]		37.73	71.35
MBPT [3]		37.76	71.33
Expt. [4]	1.383759(13)		

As a example, the energy levels and transition matrix elements of He, Be, and Mg atoms are calculated systematically. Then the static and dynamic dipole polarizabilities are further determined by the sum-over states approach. Table 1 lists the static dipole polarizabilities of the ground states of He, Be, and Mg atoms. The present RCICP results agree well with all other results [2, 3, 4]. This method and program can also be applied in the calculation of the energy levels, transition matrix elements, static and dynamic dipole polarizabilities of more complicated atoms, such as Yb, Ba, and Sr.

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