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Relativistic effects in positronic alkali atoms

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Synopsis In order to investigate interactions between a positron/positronium and an atom/ion, we calculate positronic alkali atoms, a loosely bound state of an alkali ion and a positronium, as a three-body system composed of the positron, valence electron and residual ion core within a frozen core approximation. We optimize model potentials to reproduce energy levels and fine structure splittings of alkali atoms. The ion core polarization by a positron is determined more precisely than other previous studies. We found that the relativistic effects amazingly contribute to the binding energy of the positronic alkali atom. We also discuss the rearrangement effect on the relativistic corrections and roles of positronium-ion and atom-positron configurations.

A positron (e^+) is an anti-particle of an electron, having the same mass as the electron and equal but opposite charge. In matter, the positron is located far from the nuclei of atoms/molecules by the Coulombic repulsive interaction. A positron can be bound to an atom and form a positronium (Ps), the simplest hydrogen-like atom composed of a positron and an electron. The Ps formation is one of the most important reaction of the positron and atoms/molecules as both theoretical and experimental aspects. Recently, experimental techniques to control Ps atoms have been sophisticated rapidly. An energy tunable Ps beam [1] and a QED test for the ground state of Ps [2] have been accomplished. For the more quantitative estimation of experiments treating positrons/positroniums, high-precision theoretical study on interactions between a positron/positronium and an atom are indespensable.

A positronic alkali atom is one of the ideal systems to calculate atom-positron and ion-positronium interactions because we can regard this system as a simple three-body system consisting of the positron, valence electron and residual ion core within a frozen core approximation. When a positron attaches to an alkali atom (A), the valence electron transfers to the positron and forms a Ps atom because the ionization energies of alkali atoms (around 5 eV) are smaller than the binding energy of Ps (6.7eV). The residual ion core (A^+) polarizes the Ps atom and forms a loosely bound state of the positronic alkali atom (APs^+). Although a lot of theoretical studies have been done, calculated binding energies associated with a dissosiation threhold of A^++ Ps are scattered depending on the model potential between the positron/electron and ion core introduced along with the frozen core approximation [3, 4].

In our previous work [5], we pointed out that relaivistic effects can contribute to the binding mechanism of positronic alkali atoms by a simple approximation. Since the relativistic effects are much larger in a heavy atom than those in a light atom, many previous studies focus on atomic/molecular systems containing heavy atoms. In the case of positronic alkali atoms, only Li and Na atom can bind a positron. Relativistic corrections, therefore, have been considered to be small and not calculated precisely.

In this work, we examine the model potential and its role to the binding mechanism. In order to determine the polarization potential between the A^+ and e^+ precisely, we modify the electron exchange potential by introducing dependencies of the valence electron angular momentum and the inner electron kinetic energy. Then we calculate the relativistic corrections to the binding energy of $LiPs^+$ and $NaPs^+$ within the first-order perturbation theory, based on the Breit-Pauli interactions. We found that the relativistic effects amazingly contribute to the binding energy of APs^+, as shown in table 1. We also discuss how rearrangement, namely Ps + A^+ and A + e^+ configurations, affects the relativistic corrections in the loosely bound state.

Table 1. Relativistically corrected binding energy associated with a dissosiation threhold of A^++ Ps (singlet). Effects of relativistic corrections are shown in the bottom line. All energies are given in atomic units (a.u.).

	$NaPs^+$	Na (3s)
$-\varepsilon^{\mathrm{nr}}$	0.000 472 7	0.188 566
$\Delta\varepsilon^{\mathrm{rel}}$	−0.000 032 6	−0.000 292
$-\varepsilon^{\mathrm{rel}}$	0.000 487 8	0.188 878
$1-\varepsilon^{\mathrm{nr}}/\varepsilon^{\mathrm{rel}}(\%)$	3.09	0.155

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