Calculation of positron binding to copper, silver and gold atoms

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We have developed a new relativistic method for calculation of positron binding to atoms [1]. The method combines the configuration interaction method with many-body perturbation theory. The problem of slow convergence caused by virtual positronium formation was overcome by combining several techniques. First, the atom is put in a box of finite size R_{max} with the zero boundary conditions for the wave function. Varying R_{max} controls the convergence while the effect of the finite box size on the binding energy is taken into account analytically. Second, the B-splined technique [2] is used to improve the convergence with respect to the number of radial functions in each partial wave. We included electron and positron single-particle basis states with angular momentum up to $l_{max} = 14$. Convergence was clearly achieved. We apply this method to positron binding by copper, silver and gold atoms. To test the method, we calculated electron affinities of Cu, Ag and Au. The results are summarised in the table. It was found that the copper and silver atoms form bound states with a positron while the gold atom does not. Our calculations reveal the importance of the relativistic effects for positron binding to heavy atoms. The role of these effects was studied by varying the value of the fine structure constant α. In the non-relativistic limit, $\alpha = 0$, all systems e^+Cu, e^+Ag and e^+Au are bound. Relativistic effects in electron affinities were also studied.

Table 1: Positron and electron binding energies to Cu, Ag and Au atoms (meV) (negative energy means no binding)

Atom	Positron binding energy		Electron Affinity		
	Non-relativistic	Relativistic	Non-relativistic	Relativistic	Experiment[3]
Cu	200	170	1120	1218	1236
Ag	200	123	1132	1327	1303
Au	220	-87	1369	2307	2309

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