Abstract for ICAMDATA05, Meudon, France
October 15–19, 2006

The importance of both electron correlations and relativistic effects for intermediate-Z elements

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Domain : Astrophysics

Using a modified R-matrix code, the fine-structure-resolved partial photoionization cross sections of ground and excited Na (Z=11) are calculated within the Breit-Pauli approximation, which involve bound and continuum state wavefunctions. Our calculated energy levels of Na^+ and Na agree well with the experimental values within 1%. The calculated branching ratios of the J-resolved partial cross sections of excited Na are in excellent agreement with the recent measurements[1]. Our calculated cross sections and minimum position of ground Na in the low photoelectron energy range ($<$9 eV) are in excellent agreement with the experimental results[2]. In the high energy range ($>$9 eV), there is an abnormal bump in the experimental measurements, which is a long-standing experimental puzzle[2]. It is interesting to note that there is also an absorption window in the photoabsorption (i.e. photodissociation) cross sections of Na_2^+. Such absorption window provides an answer to the puzzle. Excellent agreement between our theoretical results of Na (with Z=11) and the experimental results demonstrates that the electron correlations and the relativistic effects are treated adequately on equal footing in our calculations. Using the the bound and continuum state wavefunctions with sufficient accuracy, the relative bound-bound radiative transition rates, bound-free photoionization cross sections and electron impact cross sections, which are vitally important in relative fields, can be calculated with adequate precision. The stringently tested Breit-Pauli R-matrix code should be useful to provide the indispensable fine-structure-resolved atomic physical data of intermediate-Z elements such as C, N, O, Ne, Na, Si, S, etc., which play important roles in astrophysics.

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