Ce^{2+} jono energijos spektro ir radiacinių šuolių teorinis tyrimas

Theoretical study of energy spectra and radiative transitions of Ce^{2+} ion

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In this work, *ab-initio* atomic calculations for Ce^{2+} were performed. Ce^{2+} is one of the important candidates to produce strong absorption features in near-infrared spectra of kilonova, electromagnetic emission from neutron star mergers. GRASP2018 [1] package, based on the multiconfiguration Dirac-Hartree-Fock and relativistic configuration interaction methods, was used to compute energy levels of the ground $[Kr]4d^{10}5s^25p^64f^2$ and first excited $[Kr]4d^{10}5s^25p^64f5d$ configurations and transition data. Energy levels were compared with recommended values from the NIST Atomic Spectra Database (NIST ASD) [2] and other available works.

The influence of the correlations was studied by opening the closed shells step by step for substitutions. To reduce the computational resources, the importance of the correlations of the closed shells was studied for the levels of the ground configurations with $J = 4$ (since it is the ground level) and the levels of the first excited configuration with $J = 3$. From the analysis it follows that correlations from 4d shells are important. By opening the 4p shell the energies of the ground configuration almost do not change; the energies of the first excited configuration are too high. Restricting the substitutions from 4p and 4s shells (allowing only single substitutions) improves the agreement with the NIST data. By opening the 3d shell the agreement remains similar.

Fig. 1 presents the comparison of the final results with the NIST ASD and with other theoretical calculations. The differences between present results with NIST ASD for energy levels of two configurations till 12000 cm^{-1} energy reaches 600 cm^{-1}. The disagreement of other energies reaches 2500 cm^{-1}, and the largest difference (8200 cm^{-1}) is for the level of the ground configuration ($4f^2\ {}^1S_0$). The root-mean-square (rms) deviations obtained for energy levels of the ground configuration from the NIST data are 2732 cm^{-1} but excluding the level with worst disagreement ($4f^2\ {}^1S_0$), the rms is 1404 cm^{-1}. The rms for the first excited configuration is 618 cm^{-1}.

It should be mentioned that in [3] only some levels of the ground and first excited configurations were studied, in [4] only energy levels of the ground configuration were studied. The differences of other theoretical results with NIST data for most energy levels are similar. The rms for energy levels of the ground configuration by Froese Fischer and Godefroid from the NIST data with excluded level ($4f^2\ {}^1S_0$) is 1777 cm^{-1}. The rms for energy levels of the ground configuration by Carvajal Gallego et al. [5] from the NIST data with excluded level ($4f^2\ {}^1S_0$) is 1392 cm^{-1}, and 565 cm^{-1} for the first excited configuration. Levels of the first excited configurations computed by Safronova et al. disagree about 4000 cm^{-1}.

The transition data were also computed and evaluated. The discussion of transition data in details would be presented during the conference.

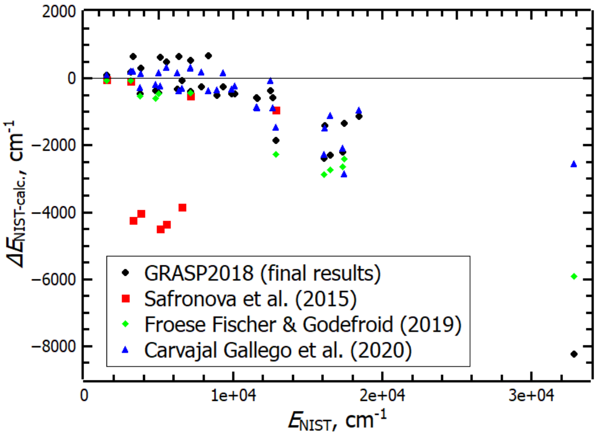

Fig. 1. Differences between NIST ASD energy levels and those of the present GRASP2018, and other calculations (in cm^{-1})

Keywords: energy levels, transition data

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