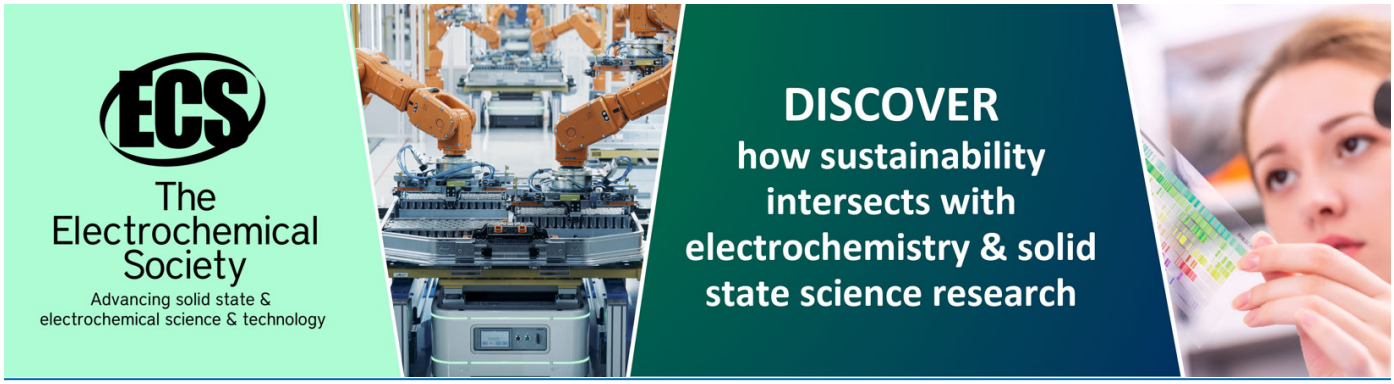
Theoretical studies of energy spectra and E1 transitions of Ni II ion



Theoretical studies of energy spectra and E1 transitions of Ni II ion

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Synopsis Accurate atomic data of the iron group elements are of major importance in astrophysics. In the present work energy spectrum calculations are performed for 332 lowest states for Ni II ion. Energy levels are compared with NIST database recommended values. All computations were done using the general-purpose relativistic atomic structure package GRASP2018.

Nickel belongs to the iron group elements, and it is one of the most abundant element from this group in cosmic objects. In the determination of abundances the accurate transition characteristics are needed. In the NIST [1] database there are not much electric dipole transition data for Ni II ion (only transitions between [Ar]$3d^9$ (ground), $3d^8 4s$, and $3d^8 4p$ configurations).

In this work the multiconfiguration Dirac-Hartree-Fock and relativistic configuration interaction (RCI) methods, which are implemented in the general-purpose relativistic atomic structure package GRASP2018 [2], were used for energy spectra computations. The transverse-photon (Breit) interaction, the vacuum polarization, and the self-energy corrections were included in the RCI calculations. Atomic state functions (ASFs) were obtained as expansions over jj-coupled configuration state functions. To provide the LSJ labeling system the ASFs were transformed using the method provided by Gaigalas *et al.* [3].

The energy spectra for 332 lowest states for Ni II ion were computed. The calculations are in progress. So here are presented the preliminary results where just valence-valence electron correlations are included. The inactive core used in the present calculations is [Ar]. For the construction of the ASFs single and double substitutions from $3d^9$, $3d^8\{4s, 4p, 4d, 4f, 5s, 5p, 5d, 6s, 6p\}$, $3d^7 4s^2$, and $3d^7 4s4p$ configurations to active orbitals set $\{7s, 7p, 6d, 5f, 5g\}$ were allowed.

In Figure 1 excitation energies of the lowest states for each configuration are compared with data from NIST [1] database. As it seen from the figure, the largest disagreements are for energy levels of $3d^8 4s$ and $3d^7 4s^2$ configurations. For other lowest states of studied configurations the difference with NIST is less than 1%, except $3d^7 4s4p$ configuration.

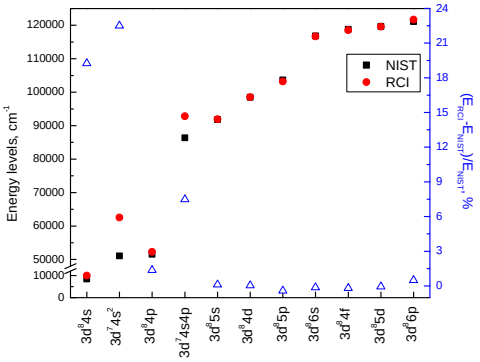

Figure 1. Excitation energy of the lowest state for each configuration. Black squares show the data from the NIST [1] while red circles show GRASP2018 results (RCI). The right Y axis and blue open triangles show the difference (in %) between RCI and NIST results for plotted states.

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