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重元素イオンエネルギー準位構造の粗視化と普遍性
Coarse-graining and universality of energy level structures of heavy element ions

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Studies on emission spectra from heavy element ions with open 4f-shells have been hot topics in many fields of sciences, *e.g.*, electromagnetic emission of r-process elements in ejecta of binary neutron star merger [1], unresolved-transition-arrays (UTAs) of tungsten and lanthanide highly charged ions in fusion [2] and laser induced plasmas [3]. However, inherently complex energy level structures of such heavy elements inhibit detailed spectral simulations.

We present our atomic structure calculations for lanthanide elements using two atomic codes, HULLAC [4] and GRASP2K [5]. Figure 1 plots differential statistical-weight distributions for two excited-state configurations of Nd II binned with a finite energy interval. Results of HULLAC and GRASP2K calculations are compared with available data in NIST ASD [6]. Although the NIST data are available only at low energies, overall profiles of the coarse-grained distributions are apparently in good agreement indicating a universal structure behind. Based on the HULLAC results, it is found that the universal structure is well depicted by the skewed normal distribution using the first three moments, *i.e.*, mean, variance, and skewness of the statistical-weight distribution. Physical properties in the energy level structures can be characterized in terms of the statistics. The skewness of the distributions for Nd II and Er II shows that their energy level structures are consistent with Hund's rule. Kolmogorov-Smirnov statistical test is applied to judge whether stochastic sampling of the energy levels leads to this heuristic skewed normal distribution. The null hypothesis is accepted for Nd II $4f^35d^2$ at the significant level of 0.05 as long as the number of sampling is not too large. We will discuss also for perspectives of facilitation of spectral simulations using the present results.

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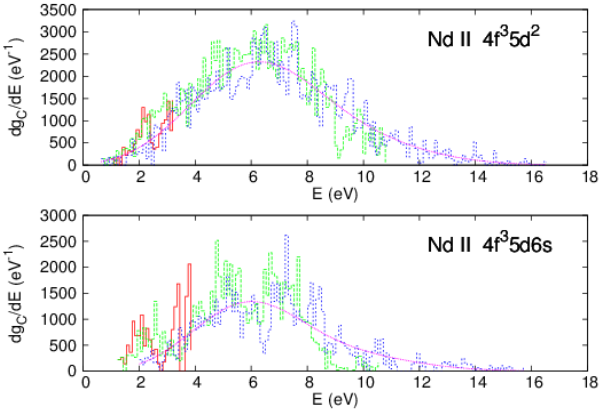

Fig. 1 Differential statistical-weight distributions of $4f^35d^2$ (upper) and $4f^35d6s$ (lower) configurations. Red color stands for NIST ASD, green GRASP2K, and blue HULLAC. The results are binned with the energy interval of 0.1 eV. Corresponding skewed normal distribution functions are plotted by purple curves. GRASP2K results are plotted up to the ionization threshold of Nd II (10.783 eV).

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