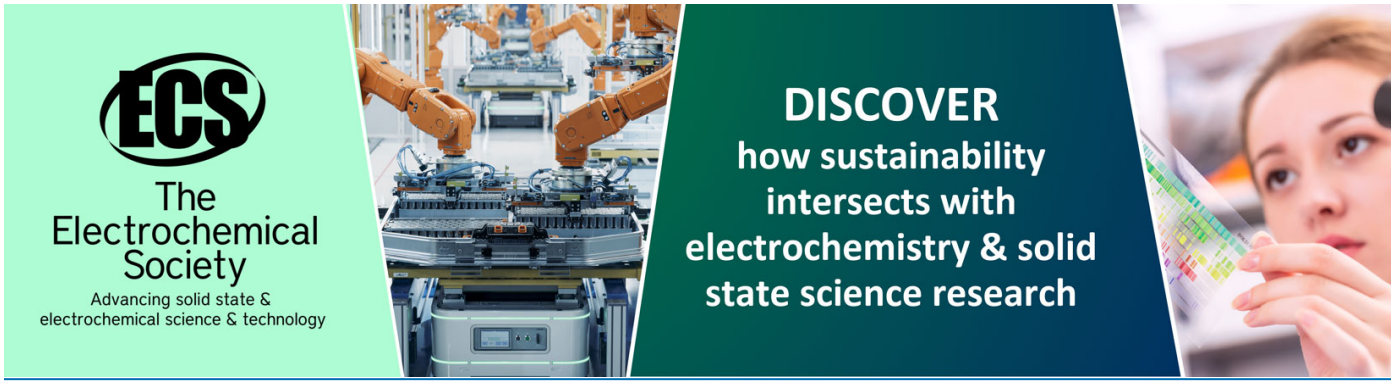
Bayesian atomic structure calculations for collisional problems



Bayesian atomic structure calculations for collisional problems

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Synopsis The calculations of collisional processes require an accurate description of the target. In general, the atomic structure is obtained through tedious iterations in which a variety of configurations and parameters are chosen to minimize the differences between the numerical and experimental values of the energies and the oscillator strengths. Using a Bayesian machine learning analysis through a Tree–structured Parzen Estimator, we can reproduce the experimental atomic structure with high accuracy. Results for neutral beryllium are presented.

The computation of collisional rates demands an accurate description of the ions involved in the processes [1]. However, the determination of an adequate atomic structure can signify lots of time and computational resources. The optimization of the target wavefunctions relies on considering a configuration interaction (CI) expansion, in which additional levels are added to improve the accuracy of the calculations. Often, the radial wavefunctions are obtained with model potentials containing scaling parameters, which are then varied. The design of automatic optimization is a challenging task. The number of configurations included in the CI, and the variation of the scaling parameters, lead to erratic oscillations in the results. This behavior implies the lack of a systematic and logic prescription for this procedure.

In this contribution, we implemented the Bayesian method via a Tree–structured Parzen Estimator from HYPEROPT [3] to optimize the atomic structure of the ions. The sequential model–base optimization turns to be an excellent machine learning methodology to minimize the scalar–valued error functions. To illustrate the procedure, we considered the neutral beryllium atom. The correct description of the target has proven to be necessary to obtain accurate electron impact excitation and electron impact ionization cross sections [4, 5].

The atomic structure of Be is calculated with the AUTOSTRUCTURE code [2], and the orbital radial wavefunctions are obtained with a Slater–type–orbitals containing λ_{nl} scaling parameters. These parameters are then optimized within a Bayesian model. The target expansion involved the $2snl$ configurations up to $nl = 5g$, and $2p^2$. We included the first six orbitals in our *search space*, and they were varied around $\lambda_{nl} = 1$. The results obtained after 10000 evaluations are given in Fig. 1. The agreement for the $2s^2\,{}^1S$, $2s2p\,{}^3P$ and $2s2p\,{}^1P$ energies with the benchmark data [6, 7] is better than 0.1%.

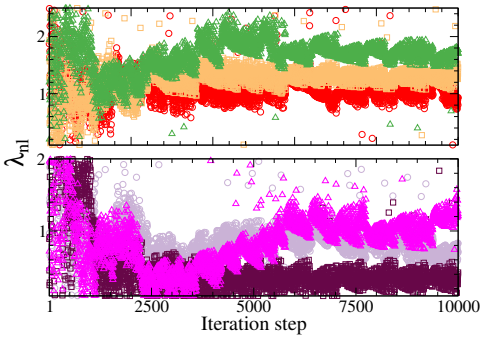

Figure 1. Bayesian optimization for the scaling parameters. Up: λ_{1s} and λ_{2l}. Down: λ_{3l}.

References

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