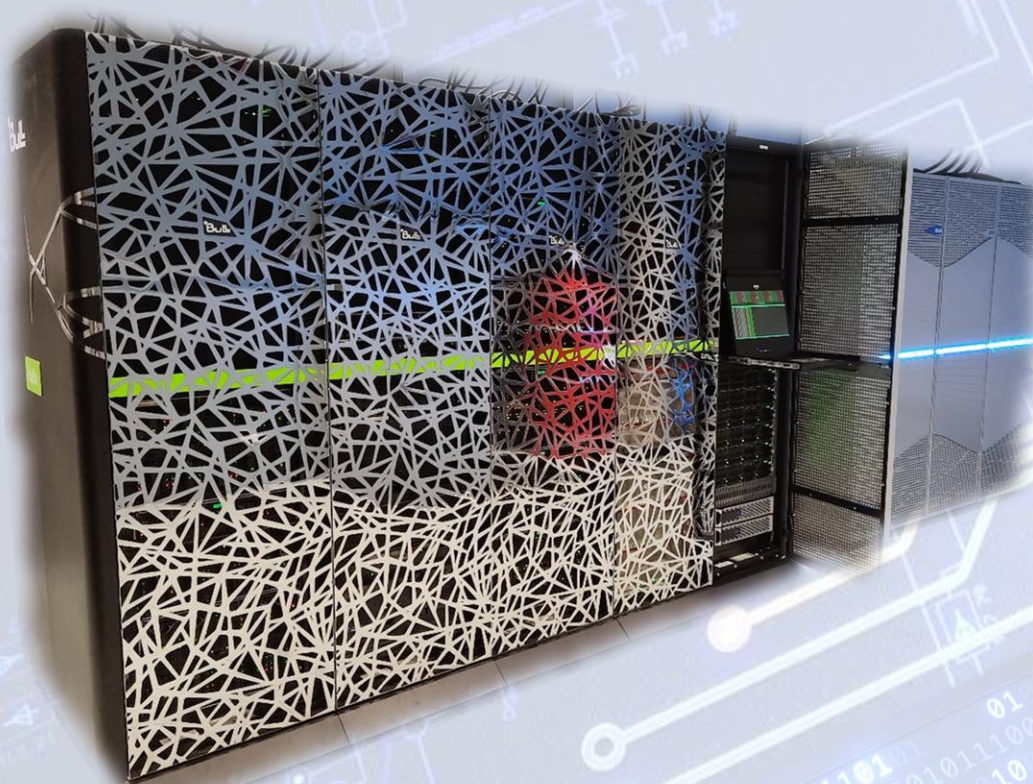




3RD EUROCC VILNIUS WORKSHOP ON USING HPC



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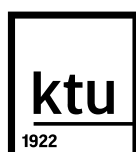
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Theoretical study of electron-impact ionization for Ne^{2+} , Ne^{3+} , and Ne^{4+}

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Electron-impact single ionization process for the Ne^{2+} , Ne^{3+} , and Ne^{4+} ions is investigated as a result of direct and indirect ionization processes. The ionization is analyzed for all energy levels of the ground configurations. The excitation-autoionization (EA) process is the strongest indirect ionization process for the studied ions. EA is initiated by electron-impact excitation to intermediate autoionizing state that subsequently decays to next charge state through autoionization process. However, the produced autoionizing state also can decay through radiative transitions, by this, reducing population of ions transferred to higher ionization stage.

The distorted wave (DW) approximation, implemented in the Flexible Atomic Code (FAC) [1], is used to study collisional ionization and excitation cross sections. Direct ionization (DI) and excitations are analyzed from the 2s and 2p subshells of the ground configurations of the neon ions. The excitations up to shells with the principal quantum numbers $n \leq 20$ are included in the study.

The scaling factors for the DW cross sections are used to explain measurements for the Ne^{2+} and Ne^{3+} ions since the DW approximation overestimates experimental data. Additionally, the single ionization threshold value provided by NIST is integrated into the study to derive the final ionization cross sections for Ne^{2+} .

The EA process accounts for $\sim 16\%$ of the total ionization cross sections from the ground state of the Ne^{2+} ion. What is more, the EA channels provide $\sim 24\%$ for the $^1\text{S}_0$ level of Ne^{2+} . For the $^1\text{D}_2$ level of Ne^{2+} , the indirect ionization process gives $\sim 21\%$.

The EA process contributes $\sim 8\%$ of the total electron-impact ionization cross sections for the ground level of the Ne^{3+} ion. Slightly higher contribution of EA is obtained for ^2D ($\sim 12\%$) and ^2P ($\sim 18\%$) terms of the ground configuration.

Our investigation of single ionization cross sections for the Ne^{4+} ion using the DW approximation shows a good agreement with experimental data for the four lowest energy levels of the ground configuration [3]. Excitations from the 2p subshell produce configurations that lie below the ionization threshold of Ne^{4+} and therefore do not contribute to the single ionization process. The indirect ionization process contributes $\sim 12\%$ to the total ionization cross sections for the ground level. The DI 2p channel remains the dominant ionization pathway across all studied ions.

REFERENCES

- [1] M. F. Gu, The flexible atomic code, *Can. J. Phys.* **86**, 675 (2008).
- [2] V. Jonauskas, Electron-impact double ionization of the carbon atom, *Astron. Astrophys.* **620**, A188 (2018).
- [3] A. Kynienė, Š. Masys, V. Jonauskas, Electron-impact ionization for Ne^{3+} and Ne^{4+} , *J. Quant. Spectrosc. Radiat. Transfer* **330**, 109224 (2025).