29 March 2025

Re: Review of the PhD Thesis by Hubert Jóźwiak "Collisions of simple molecules and atoms in fundamental studies"

The thesis by Hubert Jóźwiak is a comprehensive study of fundamental processes governing the interactions of small molecules, employing state-of-the-art computational and theoretical techniques. The work presented covers the theoretical foundations, computational methodologies, and detailed analyses of key molecular collision processes demonstrating the successful development and application of advanced quantum mechanical and semiclassical approaches to investigate a range of molecular collision phenomena. Special emphasis is made on the beyond-Voigt line-shape parameters employing state-of-the-art *ab initio* quantum scattering calculations for several key molecular systems including H_2, HD and CO. A significant portion of the work focuses on the development and implementation of novel computational techniques, enhancing the accuracy and efficiency of molecular collision simulations. The candidate has effectively leveraged high-level *ab initio* calculations and quantum scattering methodologies to extract detailed insights into state-to-state reaction dynamics. The thesis also presents a thorough benchmarking of theoretical predictions against available experimental data, demonstrating the robustness and predictive power of the employed methodologies.

The importance of the work presented in the thesis is reflected by publication of twelve papers in top peer-reviewed journal, ten of which are as the 1st author, reporting several important scientific achievements, summarised as follows.

- The development of improved theoretical models for describing inelastic and reactive collisions, incorporating sophisticated potential energy surfaces, and advanced dynamical treatments, enhancing the accuracy of describing inelastic and reactive collisions.
- Analysis of spectral lines in planetary atmospheres, through the development of the "beyond-Voigt" contributions of small molecules, crucial for accurate interpretation of spectral data from gas giants.
- Achieving unprecedented accuracy in application of quantum scattering techniques to study complex collisional systems with impressive sub-percent agreement between purely theoretical spectra derived from these calculations and experimental spectra thus validating the accuracy of *ab initio* calculations and demonstrating a significant milestone in the field.
- The development of a custom scattering code (BIGOS), allowing overcoming limitations in existing software MOLSCAT and enabling more efficient and accurate calculations, especially for complex molecular systems, and representing a substantial advancement in computational tools for molecular collision studies.
- A detailed study of hyperfine and Zeeman effects and their implications for molecular line shapes, shedding new light on processes relevant to atmospheric chemistry, astrophysical environments, and ultracold molecular physics. High-quality comparisons

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with experimental results confirm the validity of the theoretical approaches and providing valuable insights into underlying physical mechanisms.

The BIGOS package is an especially impressive result of Hubert Jóźwiak's PhD work, enabling users to obtain accurate line-shape parameters through solution of quantum scattering equations. This custom scattering code developed by the candidate demonstrates the expertise in advanced computational techniques, implementing and improving state-of-the-art methods for molecular collision studies. The new computational methodology and underlying calculations not only advance the current understanding of molecular collision dynamics but also establish a strong foundation for future studies in the field. The research presented in the thesis is of exceptional quality, demonstrating a profound understanding of the field and an ability to push the boundaries of existing theoretical approaches.

To conclude, the thesis represents a major achievement in the theoretical study of molecular collisions of small molecules, making substantial contributions to the field. The candidate has demonstrated exceptional research abilities, technical proficiency, and scientific creativity. The work presented in the thesis is based on original contributions to the field, such as the development of novel methodologies and insightful interpretations of complex molecular interactions. The thesis is well-written, with a clear presentation of theoretical concepts, computational methods, and scientific results demonstrating a high level of originality and scientific maturity. The findings have significant implications in areas beyond the field of the theory of molecular collisions, including fundamental physics, chemical reaction dynamics, astrophysical chemistry, and ultracold molecular physics. The results are highly impactful and relevant, with strong potential for further advancements in molecular collision theory.

Based on the quality of the research, the depth of the analysis, and the clarity of presentation, I strongly recommend that Hubert Jóźwiak be awarded the PhD degree with the highest distinction.

Achievements presented in the thesis certainly meet the conditions specified in Art. 187 of the Law on Higher Education and Science.

Sincerely yours,

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