PLATAN 2024 - Merger of the Poznan Meeting on Lasers and Trapping Devices in Atomic Nuclei Research and the International Conference on Laser Probing



Contribution ID: 178

Type: Poster Presentation

High Accuracy Calculations of Properties of Heavy Atoms and Molecules

Probing the properties of heavy atoms and molecules to ever greater accuracy provides ample opportunity for advancements in our understandings nuclear structure and to further extend the limits of atomic structure calculations [1-2]. In heavy atoms and molecules the role of relativistic and correlation effects are of great importance and their study adds to our understanding of these effects [3]. Numerical methods such as Fock space couple cluster, configuration interaction (CI) and CI combined with many-body perturbation theory are at the forefront of high accuracy atomic calculations. In this work calculations of properties of heavy atoms and molecules are carried out using highly accurate and relativistic numerical methods.

[1] Blaum et al., Phys. Scr. 2013, 014017 (2013)

[2] Porsev et al, Phys. Rev. Lett. 127, 253001 (2021)

[3] Dzuba et al., Phys. Rev. A. 90, 012504 (2014)

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Session Classification: Poster Sessions