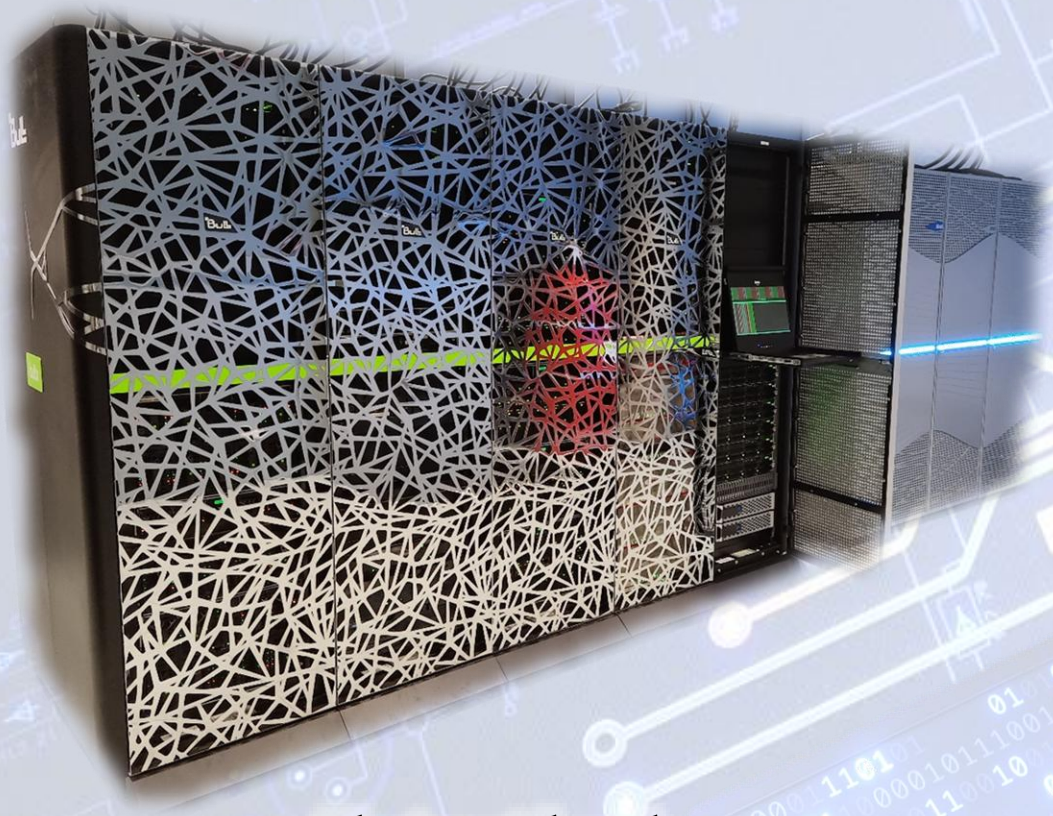
3RD EUROCC VILNIUS WORKSHOP ON USING HPC



Abstract book

https://doi.org/10.5281/zenodo.14748386

January 20–21, 2025

Vilnius, Lithuania

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Funding

Co-funded by the European Union

EuroHPC Joint Undertaking

Funded by the European Union. This work has received funding from the European High Performance Computing Joint Undertaking (JU) and Germany, Bulgaria, Austria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, France, Netherlands, Belgium, Luxembourg, Slovakia, Norway, Türkiye, Republic of North Macedonia, Iceland, Montenegro, Serbia under grant agreement No 101101903.

Bendrai finansuoja Europos Sąjunga

Projektas bendrai finansuojamas 2021–2027 metų ES fondų investicijų programos (sutartis Nr. 10-051-P-0001).

EuroCC2-EuroCC4SEE
Project Organiser

Vilniaus universitetas 1579 Universitas Vilnensis

Project Implementers

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Vilniaus universitetas 1579 Universitas Vilnensis — Matematikos ir informatikos fakultetas

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VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Modeling and investigation of high-energy materials

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The global market for high-energy materials has been consistently growing [1]. Between 2017 and 2022, it expanded from nearly USD 23.8 billion to USD 31.2 billion, and in 2024, the global explosives market reached a volume of approximately 16.58 million metric tons [2]. This growth is primarily driven by the use of these materials in mining, quarrying, and construction industries. From a practical perspective, an energetic compound should be powerful, stable, insensitive to mechanical stimuli, and capable of releasing a substantial amount of energy during intentional detonation. Consequently, the development of new functionalized compounds with unique and improved properties is essential for advancing energetic materials.

In this context, we conducted studies on various high-energy compounds with the goal of creating new materials or modifying existing ones, as well as understanding their potential risks. Our research employed Becke's three-parameter hybrid functional approach with non-local correlation provided by Lee, Yang, and Parr, combined with the cc-pVTZ basis set. This approach was used to evaluate the influence of substitutions or the formation of salts on the energetic properties of nitramines. The geometry, total energy, and heat of formation of the selected stable conformers of various materials were calculated to derive key parameters such as density, resistance to shock stimuli, detonation pressure, and velocity.

The results of our study allow us to predict new multipurpose energetic materials that achieve a good balance between energy and stability. For example, our findings indicate that compounds such as *N*-(2-nitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,4,6-trinitrophenyl)-*N*-[(3,4,5-trinitro-1*H*-pyrazol-1-yl)methyl]nitramine, *N*-(2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,2,2-trinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, and *N*-(trinitromethyl)-*N*-(2,4,6-trinitrophenyl)nitramine exhibit superior explosive properties and greater stability compared to tetryl, although they remain sensitive to shock stimuli. Based on these results, we recommend new tetryl analogs containing dinitroethyl, trinitroethyl, and trinitromethyl substituents for practical applications. Additionally, we investigated the properties of some 5-amino-3-[(2,4,6-trinitrophenyl)amino]-1*H*-1,2,4-triazole (APATO) cationic salts. The results of the energetic characterizations revealed that the synthesized salts possess enhanced energetic properties, outperforming TNT. Notably, the APATO perchlorate salt warrants special attention as a thermostable high-energy material.

REFERENCES

[1] J. Akhavan, *The Chemistry of Explosives*, 4th ed.; RSC: London, UK, (2022).
[2] Global Explosives Market Report and Forecast 2025-2034.