

Number of project:

GUKPOST/11/2024

Name of the project:

In silico study of the structure, stability and reactivity of mercury complexes in the biosphere.

Abstract:

The goal of the project is to deepen our understanding of the role of mercury in molecular complexes of biological importance (e.g., various alkylmercury species or complexes with amino acids) and their reactivity towards oxidants like OH, NO_x, SO₂ in ecosystem, addressing a critical knowledge gap in environmental chemistry. Recent findings on Hg distribution at the 2011 meeting of the International Conference of Mercury as a Global Pollutant in Halifax, Canada revealed alarming levels of mercury in the air, land, sea and living organisms. The proposed objectives exhibit a high level of quality and adequacy of the research at molecular level and aims to provide reliable molecular data on these complexes within accurate computational protocol and attaining chemical accuracy (± 4 kJ/mol)). The relevance of these objectives is undeniable, given the environmental and health implications of mercury deposition in living matter. Furthermore, this project is employing advanced in silico computational chemistry methodologies. It offers a well-considered approach for studying the properties of mercury complexes (methylmercury (MeHg), ethylmercury (EtHg), Hg-(SH), and/or HgX (X = H, C, N, O, P, S)) combining quantum chemical wave-function methods with carefully chosen density functional theory. The proposed methodology is not only appropriate but also highly relevant to the project's objectives. It comprises computational modelling and molecular simulations, aligning perfectly with the study's focus on the structure, stability, and reactivity of mercury complexes in the environment.