Contribution ID: **16** Type: **not specified**

Comparative DFT Study of Adsorption of Superheavy Elements Cn and Fl, and Their Lighter Homologs Hg and Pb on Selenium Surface

Tuesday 25 November 2025 16:10 (20 minutes)

In this computational study, we investigate the adsorption of superheavy elements Copernicium (Cn) and Flerovium (Fl), and their lighter homologs Mercury (Hg) and Lead (Pb), on a Selenium (100) surface. Our approach employs periodic Density Functional Theory (DFT) in Quantum ESPRESSO (open-source suite of codes)with spin-orbit coupling and DFT-D4 dispersion correction. Our resultsshow that while a standard Perdew-Burke Ernzerhof (PBE) setup (functional and pseudopotential) captures the correct adsorption trend, a hybrid approach using the Perdew-Burke-Ernzerhof for solids (PBEsol) functional with PBEsol pseudopotentials for Se and PBE pseudopotentials for the adsorbates provides superior accuracy for adsorption energy values. We further probed the adsorbate-surface interactions and stability through density of states, charge transfer, and vibrational analysis.

Presenter: SEN, Dipayan (Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research)