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Precision calculation of polarizability of heavy ions and atoms for physisorption with 2D materials

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The calculations of different properties of the atoms and ions play a crucial role in many applications of various fields for instance, atomic physics, material science, astronomy, plasma, nanotechnology etc. An accurate description of different atomic properties is highly challenging with the standard approximations resulting in failure in providing the good data. Therefore, the surge for accurate calculation of atomic properties has emerged from last decade using promising theoretical methods. Here, in this paper, we have evaluated one of the most important atomic property i.e., dipole polarizability of heavy ions - Zn^+, Cd^+, Hg^+, Pb^+ and atoms – Zn, Cd, Hg and Pb using two different relativistic many body methods. The known dynamic dipole polarizability values at imaginary frequencies are then used to derive characteristic van der Waal (vdW) dispersion coefficients with two dimensional (2D) materials - graphene and carbon nanotube walls, essential for physisorption applications. The agreement of the calculated dispersion coefficients is satisfactory with the recent study conducted using density functional theory (DFT) for the case of graphene. The present work is useful in sensing and storage applications of heavy elements with the considered 2D material walls. The future aspect of this work includes the accurate modelling of vdW correction based on inclusion of the higher-order coefficients which can be used to procure a higher accuracy towards total vdW potential between element and material wall.

Presenter name

Harpreet Kaur

Primary authors: Ms KAUR, Harpreet (Guru Nanak Dev University); Dr ARORA, Bindiya (Guru Nanak Dev University)

Presenter: Ms KAUR, Harpreet (Guru Nanak Dev University)

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