QUANTUM CHEMICAL AND MOLECULAR DYNAMICS SYNERGISM IN STUDYING 2D MATERIALS AND POLYMER MATRICES

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Sizes of chemical systems and their targeted properties are among the factors contributing to final decisions on levels of theory used to theoretically study chemical systems. Obviously, quantum chemical methods and molecular dynamics (MD) simulations are two general popular levels of theory frequently used to study chemical systems. In this talk, the synergism between density functional theory (DFT) and MD simulations will be demonstrated in two cases of study: i) interaction between biomolecules and MoS_2 2D materials in aqueous media, and ii) optical properties of thermal imaging polymers. In the first case, a new MD force field successfully developed based on highly accurate data obtained from DFT calculations and its application in simulations of 2D MoS_2 exfoliation mediated by peptides shall be discussed. In the second case, the use of DFT in investigation of IR spectroscopic features of a polymer family with the assistance of MD simulations in construction of 3D crosslinked polymer matrices will be presented.

References:

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