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15 January 2025

Molecular and Electronic Dynamics at Different Time Scales by Density Functional Theory

Dynamics are at the core of nearly all natural processes, with their timescales serving as a key factor in determining the appropriate microscopic approaches for their study. In this work, we employ atomistic simulations at the density functional theory (DFT) level to investigate phenomena spanning twenty orders of magnitude in time. Using ab initio molecular dynamics (AIMD), we explore interfacial transport processes of water and hydrophobic solutes on van der Waals bilayers and heterostructures, providing fundamental insights into the mechanisms governing diffuse-osmotic flow. To access longer timescales, metadynamics is employed to enhance sampling, revealing the dynamic equilibrium of adsorbates at oxide and metallic surfaces on the picosecond scale. Finally, electronic charge dynamics induced by core-level excitations are examined using real-time time-dependent DFT (RT-TDDFT), uncovering intriguing charge transfer processes in condensed matter systems. Together, these approaches provide a comprehensive framework for understanding dynamic phenomena across vastly different timescales.

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