Synergistic integration of organic molecules into two-dimensional materials: A comprehensive exploration of MoS_2/Perylene hybrid systems

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Abstract

The integration of organic molecules into two-dimensional (2D) materials marks a transformative advancement, expanding the realms of processes within the two dimensions and van der Waals (vdW) heterostructures. This synergistic alliance leverages the finite 2D materials found in nature, seamlessly merging with a diverse array of purposefully designed organic molecules. Despite the immense potential, the ability to tailor and synthesize molecules with predictable properties remains virtually boundless [1]. Organic compounds, recognized for their high absorption capabilities but limited mobility and charge stability, present a sharp contrast to inorganic compounds characterized by relatively low absorption yet outstanding charge transport properties [2]. The strategic formation of van der Waals (vdW) heterostructures, harmonizing inorganic compounds with organic molecules, holds the promise of synergizing the advantageous characteristics of both material classes. Notably, Molybdenum disulfide (MoS_2), a distinguished member of transition-metal dichalcogenides (TMDs), stands out as an exceptionally promising 2D semiconductor for applications in transistors, optoelectronics, and catalysis. Conversely, Perylenes, widely used as dyes, offer tunable optical properties through chemical modifications of their core. This study systematically explores the structural, electronic, and optical characteristics of MoS_2/perylene hybrid systems using density functional theory, incorporating various perylenes like perylene diimide (PD), perylene orange (PO), and perylene red (PR). The investigation highlights the capacity for precise fine-tuning of properties within the hybrid system, providing insights into the intricate interplay between MoS_2 and perylenes, including the effects of strain. This elucidation sheds light on the synergistic effects, paving the way for advanced applications across diverse fields and contributing to a broader understanding of 2D material integration and the customization of materials for specific functionalities.

References

[1] Y L Huang et al, JChem Soc Rev, 47(2018) 3241-3264.
[2] S M Obaidulla et al, Advanced materials interfaces, 7(2020) 1901197

Figures

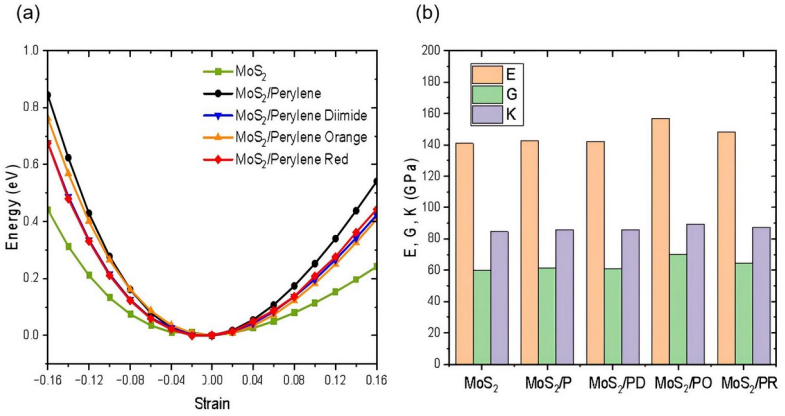

Figure 1: (a) Uniaxial strain-dependent potential energy variation, (b) mechanical properties in MoS_2/Perylene derivative interfaces.