Investigating integration of perylene derivative molecules with monolayer MoS_2: Insights into hybrid interface properties

Mohammed EL Amine Miloudi, Oliver Kühn
Institute of Physics, University of Rostock, Albert-Einstein-str. 23-24, 18059 Rostock, Germany

Oliver.kuehn@uni-rostock.de

Integrating organic molecules with two-dimensional (2D) materials represents a transformative advancement, expanding processes within two dimensions and facilitating van der Waals (vdW) heterostructures. This synergistic alliance harnesses the unique properties of finite 2D materials found in nature, seamlessly merging with a diverse array of purposefully designed organic molecules. Despite their immense potential, the ability to tailor and synthesize molecules with predictable properties remains virtually boundless [1]. Organic compounds, renowned for their high absorption capacities yet limited mobility and charge stability, starkly contrast with inorganic compounds known for relatively low absorption but exceptional charge transport properties [2]. The deliberate assembly of van der Waals heterostructures, combining inorganic compounds with organic molecules, holds promise for synergistically exploiting the advantageous characteristics of both material classes. Molybdenum disulfide (MoS_2), a prominent member of transition-metal dichalcogenides (TMDs), is a highly promising 2D semiconductor for transistors, optoelectronics, and catalysis applications. In contrast, widely utilized as dyes, perylenes offer tunable optical properties through modifications to their core structure. This study systematically investigates the structural, electronic, and optical features of MoS_2/perylene hybrid systems employing density functional theory (DFT), incorporating diverse perylenes such as perylene diimide (PD), perylene orange (PO), and perylene red (PR). The research emphasizes the precise modulation of properties within the hybrid system, providing insights into the intricate interplay between MoS_2 and perylenes, including strain effects. This elucidation sheds light on synergistic effects, paving the way for advanced applications across diverse disciplines and contributing to a deeper comprehension of 2D material integration and the tailored design of materials for specific functionalities.

References

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[2] Obaidulla, Sk Md and Habib, Mohammad Rezwan and Khan, Yahya and Kong, Yuhan and Liang, Tao and Xu, Mingsheng, *Advanced Materials Interfaces*, 7 (2020) article 1901197.

Figures

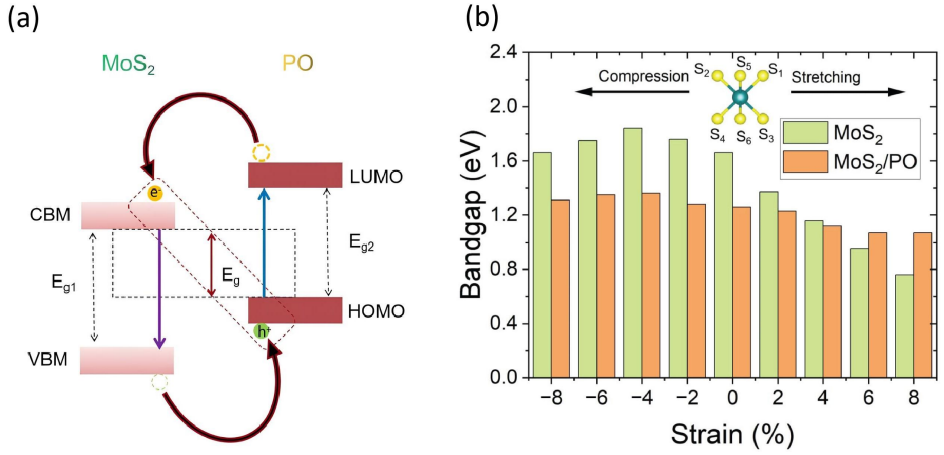

Figure 1: (a) Schematic of interface band alignment relative to Fermi energy (E_F), and (b) evolution of band gap (E_g) in strained MoS_2 and MoS_2/PO systems.