

## **Intercalation of DNA Nucleobases inside Bilayer Graphene and Bilayer MoS<sub>2</sub>: A Comparative DFT Study**

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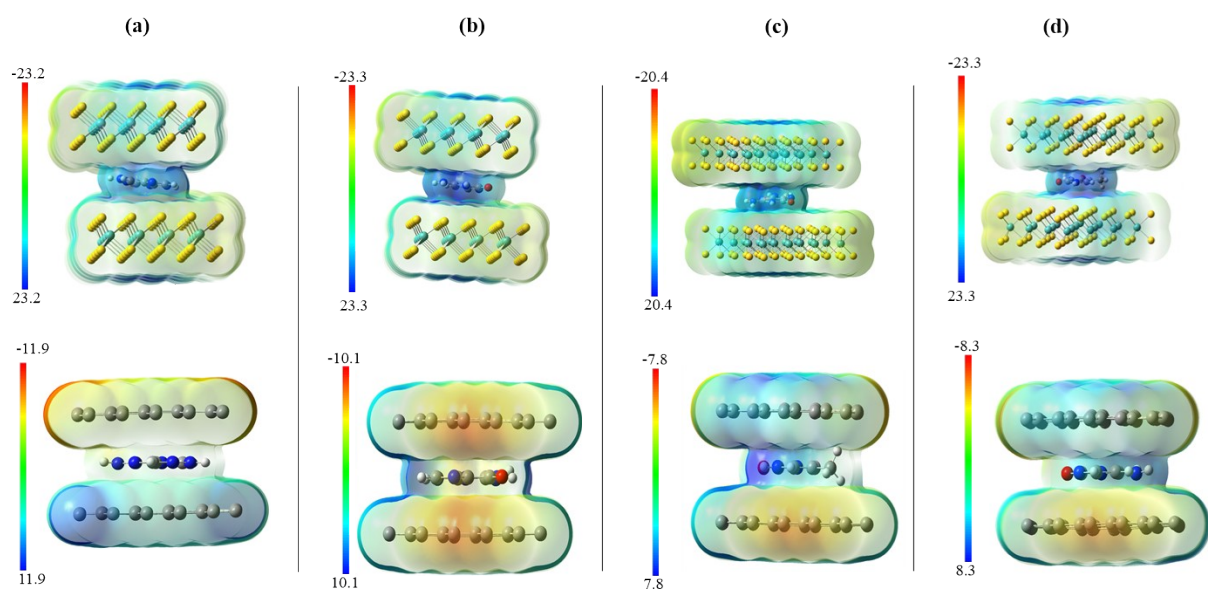


Fig. S1. (I) MESP of BL MoS<sub>2</sub> and BLG surface model and DNA nucleic bases (**a** adenine, **b** cytosine, **c** guanine, and **d** thymine) using the M062X/6-31G\* level of theory

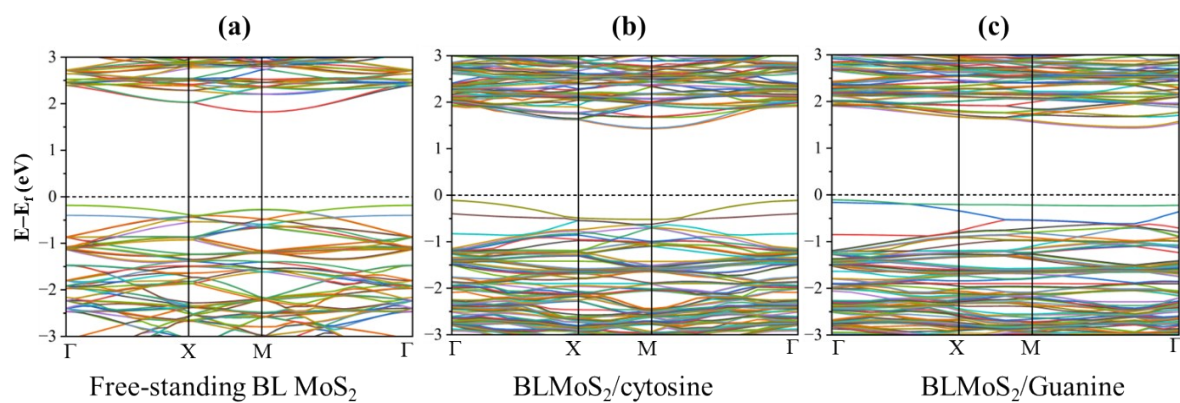


Figure S2. Total electronic band structure of (a) BLMoS<sub>2</sub> and BLMoS<sub>2</sub>-nucleobase complexes with (b) cytosine, and (c) guanine.