Electronic state tuning of WS_2 by sumanene adsorption

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Atomic layer materials can form hybrid structures with foreign materials. In such complexes, guest materials highly modulate the electronic structures of host atomic layer materials, irrespective of their interactions. Bowl-shaped hydrocarbon molecules, sumanene and corannulene, are unique guest materials for the atomic layer materials to which those molecules modulate the Fermi level energy owing to their dipole moment. Sumanene and corannulene intercalated in bilayer graphene cause charge redistribution in the graphene layers, leading to the multi-carrier system in bilayer graphene [1,2]. In this work, we aim to investigate the electronic structures of WS_2 adsorbing sumanene columns [Figs. 1(a) and 1(b)] in terms of column orientation and length, using density functional theory with an effective screening medium method.
Our calculations show that sumanene columns modulate the electronic structures of WS_2, because of their dipole moment. The valence and conduction band edges of WS_2 monotonically shift downward with the increase of the column length when the columns are adsorbed on WS_2 in the concave arrangement. In contrast, the band edges of WS_2 shift upward with the increase of the column length when the columns are in the convex arrangement. These results imply the possibility of the band engineering of transition metal dichalcogenides by controlling the adsorbates' arrangement and species.

References

[1] M. Maruyama and S. Okada, ACS Appl. Nano Mater. 4 (2001) 3007.
[2] M. Maruyama and S. Okada, J. Appl. Phys. 131 (2022) 134303.

Figure

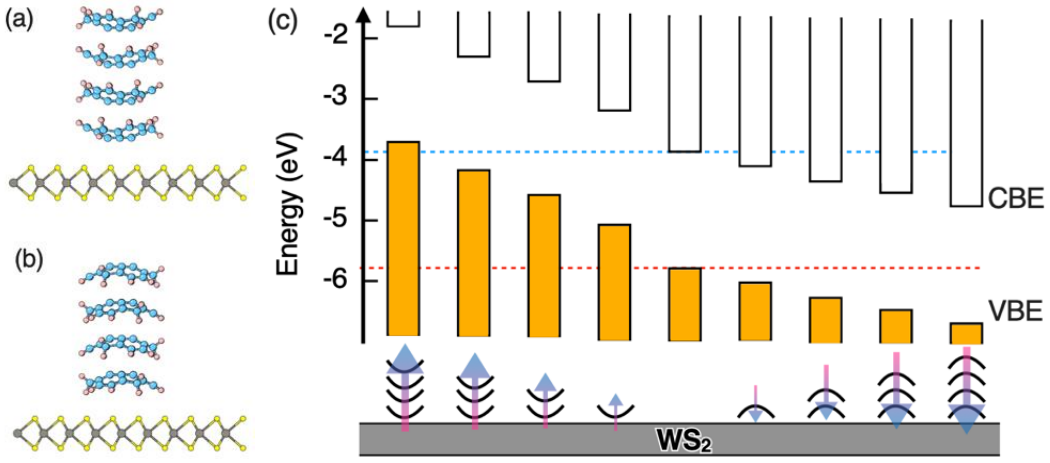

Figure 1: Geometric structures of WS_2 adsorbing sumanene columns with (a) convex and (b) concave molecular conformations. (c) Kohn-Sham energies of the valence and conduction band edges of WS_2 by sumanene adsorption regarding column length and molecular conformation. Energies are measured from that of the vacuum level. CBE and VBE indicate the conduction and valence band edges.