Supporting Information

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Stacking stability and sliding mechanism in weakly bonded 2D transition metal carbides by van der Waals force

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To test the effect of different functional on the potential energy surface (PES), we have calculated the PESs of the Ti_2CO_2-I complementing the vdW-DF2, rev-vdW-DF2, and without considering vdW correction, respectively, as shown in Fig. S1. We found that the energy barrier difference between vdW-DF2 and rev-vdW-DF2 is very small (vdW-DF2: 0.112 eV, rev-vdW-DF2: 0.122 eV), while there is a significant difference between the PES with vdW and that without vdW. Thus, it would indicate that the species of functional does not affect significantly sliding energy barriers for this systems that much.

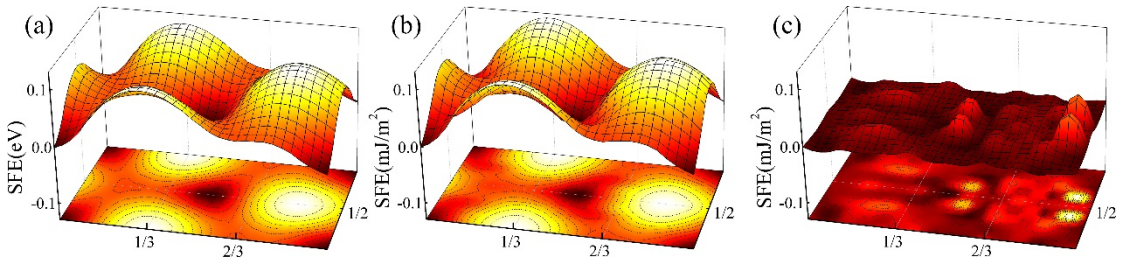

Fig. S1 The corresponding PES of the Ti_2CO_2-I as a function of relative displacement of the two layers in the *x* and *y* directions complementing the vdW-DF2 (a), rev-vdw-DF2 (b), and without vdW (c), respectively.

We also tested the effect of strain on the energy barrier complementing the vdW-DF2 and rev-vdw-DF2, respectively. We took *x*-axial strain as a representative. As shown in Figure S2, the energy barrier using rev-vdW-DF2 is a little higher than that using vdW-DF2. The reason is that vdW-DF2 systematically overestimates layer separations so that energy barrier is underestimate. No matter whether adopting vdW-DF2 or rev-vdW-DF2, their energy barriers increase with increasing strain. Therefore, different functional give similar predictions, indicating that exchange does not affect the sliding barrier that much.

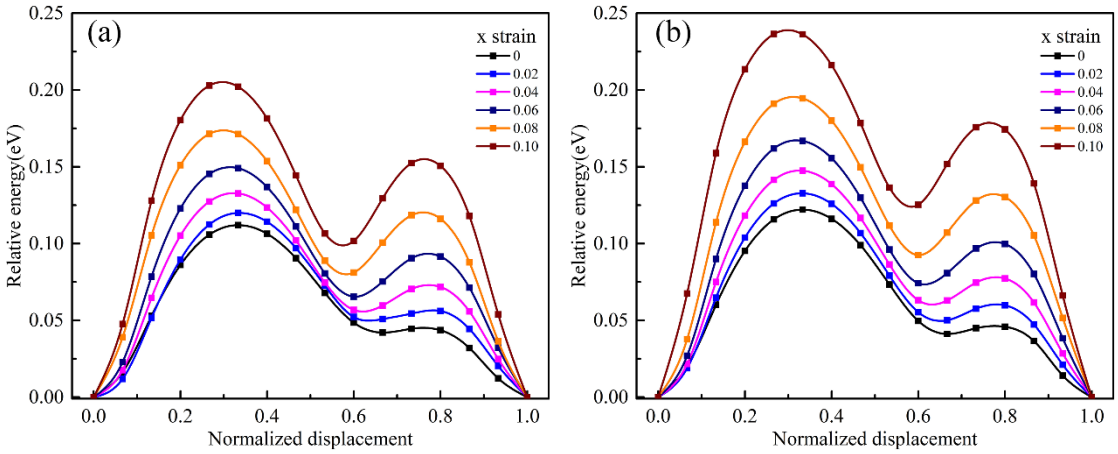

Fig. S2 The x-axis sliding potential energy profiles under *x*-axial strain complementing the vdW-DF2 (a) and rev-vdw-DF2 (b), respectively.

We test the energy of Ti_2CO_2-I using Γ-centered Monkhorst-Pack grid of 12×20×1, 12×20×2, and 12×20×3, respectively. As shown in Fig. S3, the energy difference among them is less than 0.001eV. Therefore, 3 points in *z* direction are a little redundant but do not affect the results.

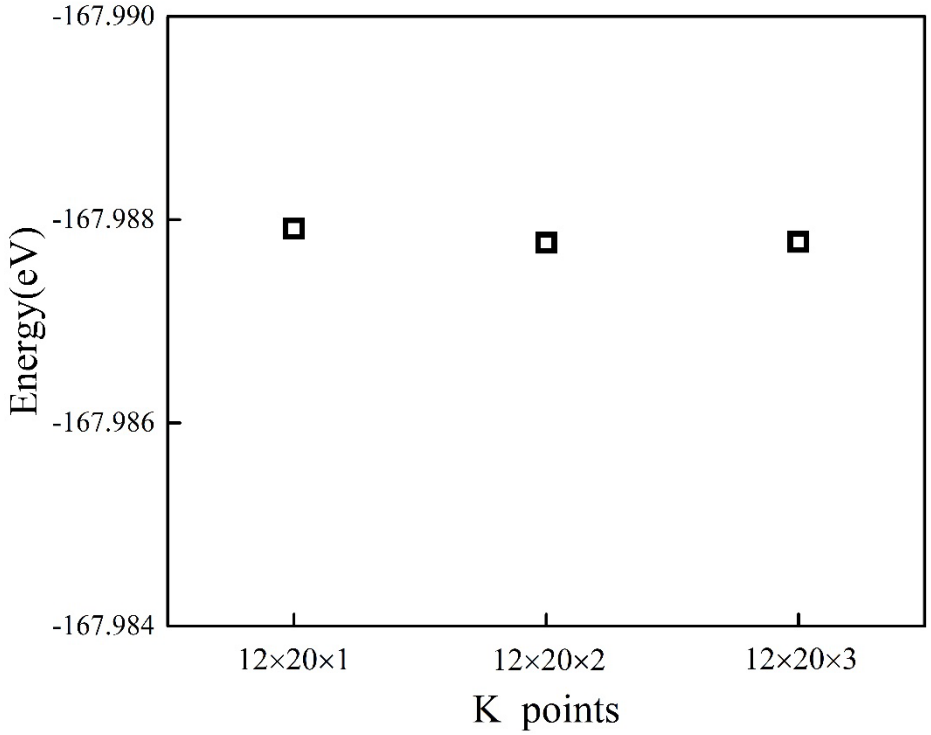

Fig. S3 The energy of Ti_2CO_2-I using Γ-centered Monkhorst-Pack grid of 12×20×1, 12×20×2, and 12×20×3, respectively.

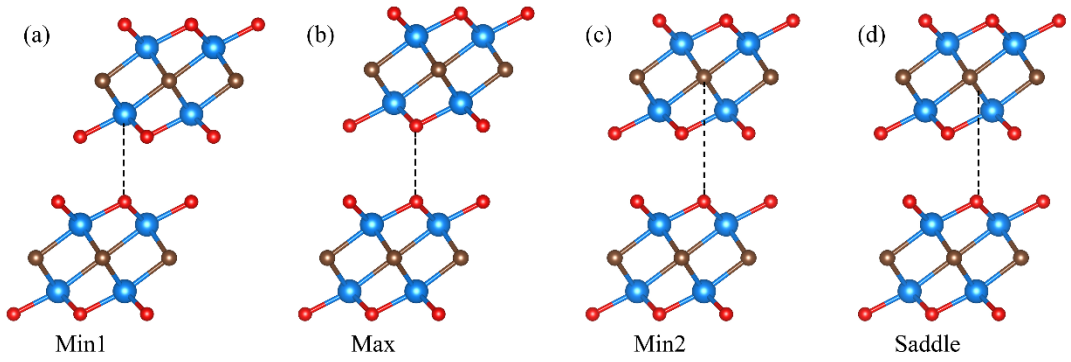

Fig. S4 Geometric arrangement for the most relevant positions (Min1 (a), Max (b), Min2 (c), and Saddle (d)) along the profiles.

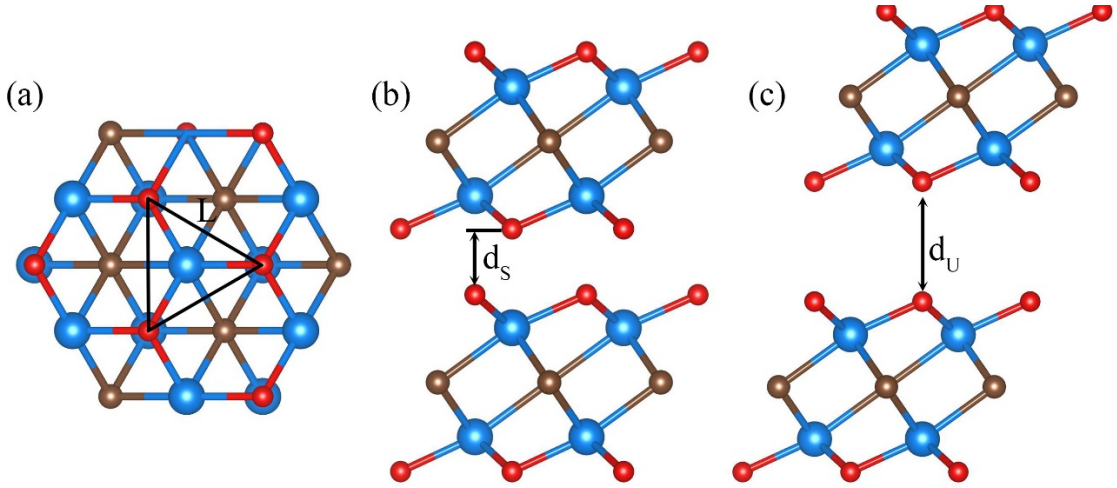

Fig. S5 Top view of bottom layer of bilayer M_2CO_2 (a). The triangle in (a) is a hollow. Side view of bilayer M_2CO_2 at Min1 (b) and Max (c). *L* represents the in-plane oxygen distance, and d_S represents the layer distance at Min1, and d_U represents the layer distance at Max. Layer distance is the *z* distance of the closest atoms in two layers.

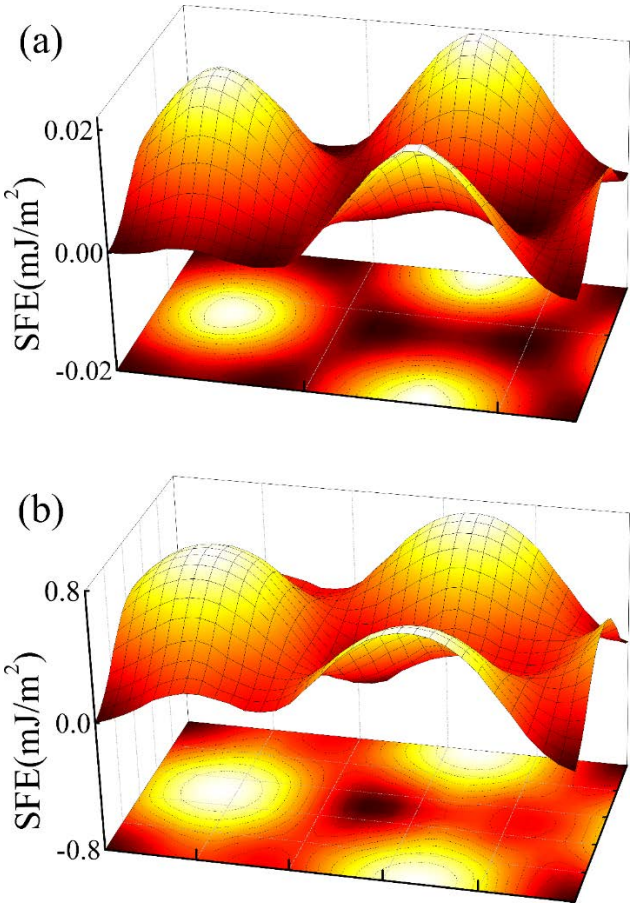

Fig. S6 The corresponding potential energy surface (PES) of the graphene (a) and Ti_2C (b) as a function of relative displacement of the two layers in the *x* and *y* directions.

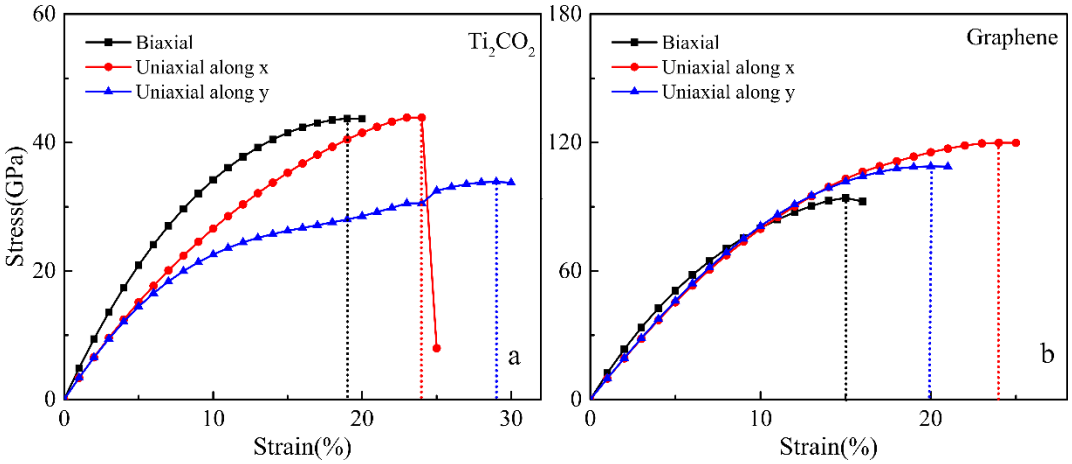

Fig. S7 The strain-stress relations for Ti_2CO_2 (a) and graphene (b) under both biaxial and uniaxial load conditions.

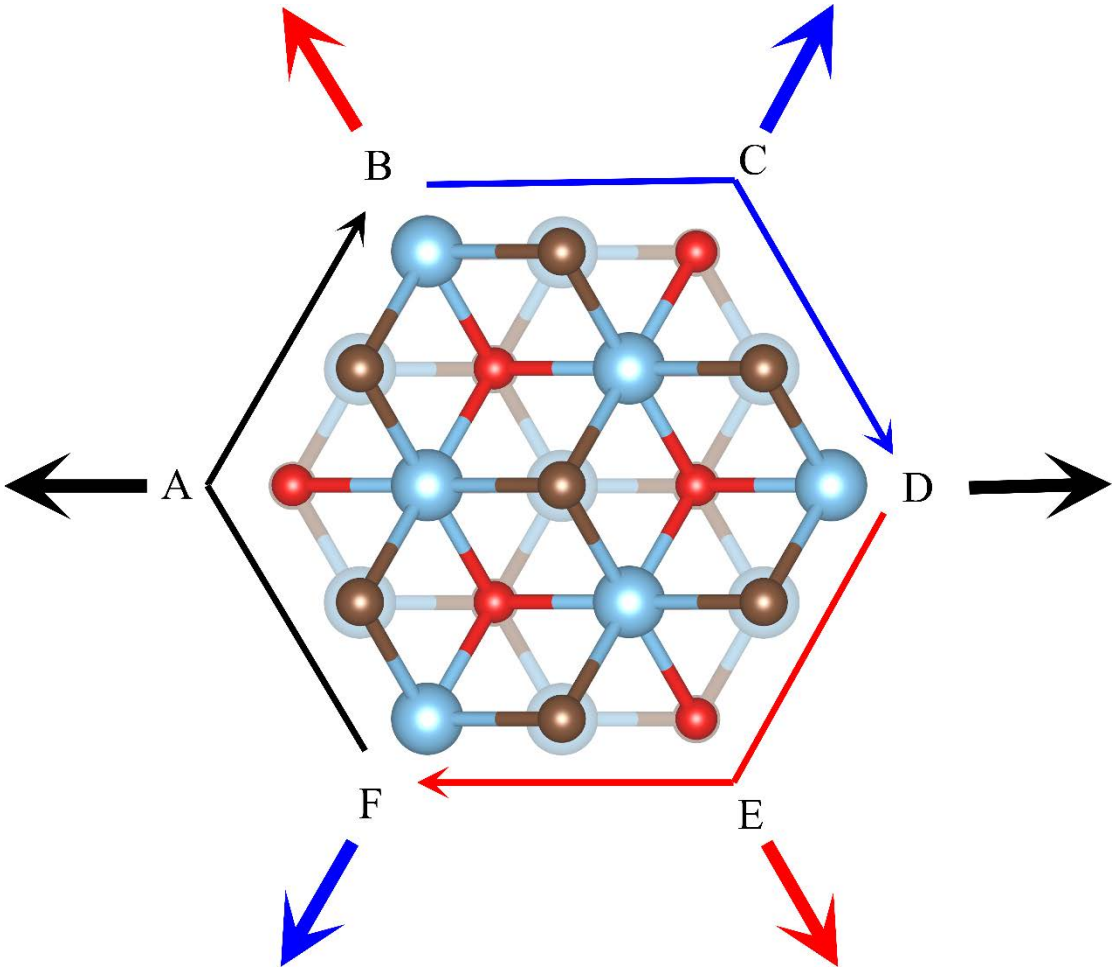

Fig. S8 Different tensile directions and corresponding MEPs.