

Supporting Information

Intrinsically Substitutional Carbon Doping in CVD-Grown Monolayer MoS₂ and the Band Structure Modulation

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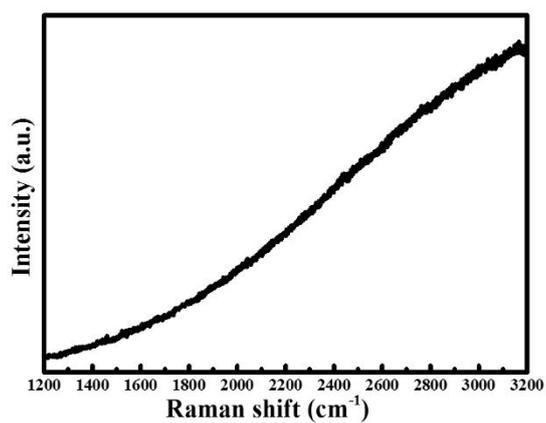


Figure S1. Raman spectrum of the carbon doped monolayer MoS₂ showing that no deposition of amorphous carbon or graphene formed.

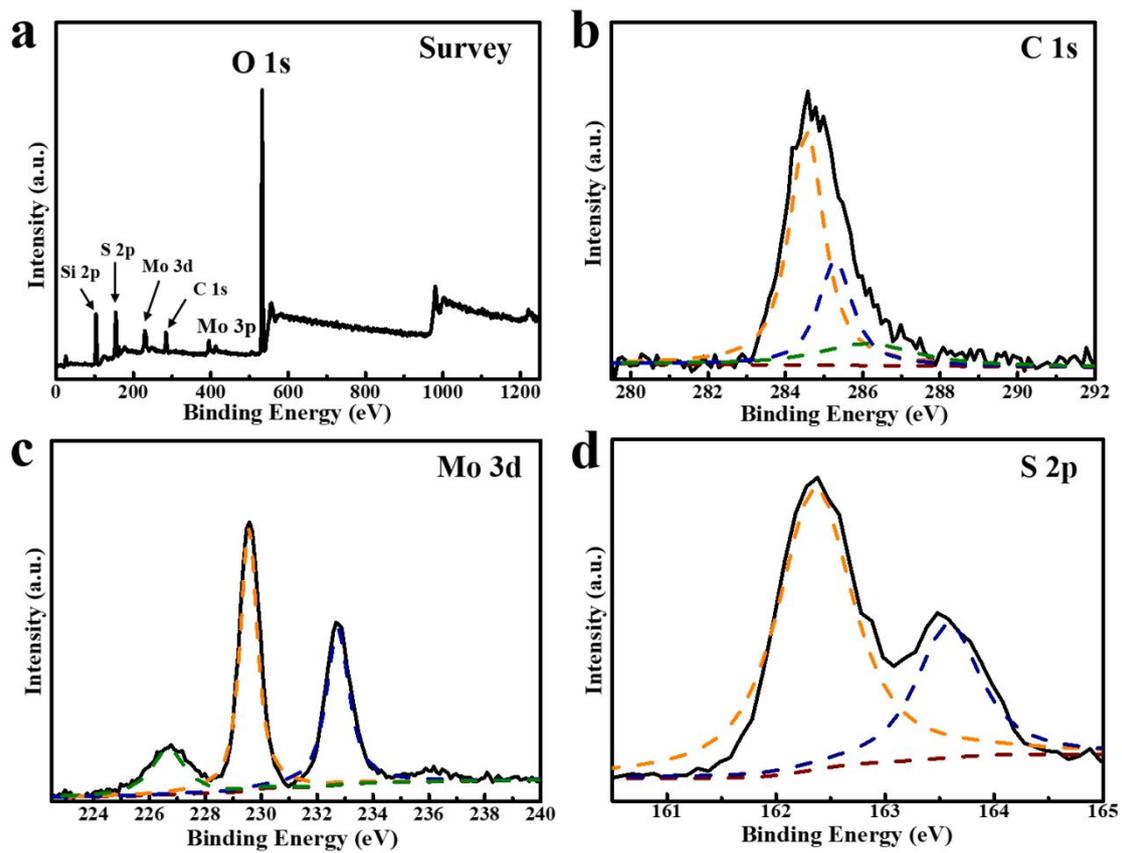


Figure S2. XPS characterization of the growth samples with 99.999% purity MoO_3 precursor. (a) The survey scan. (b-d) C 1s, Mo 3d, and S 2p core-level binding energies.

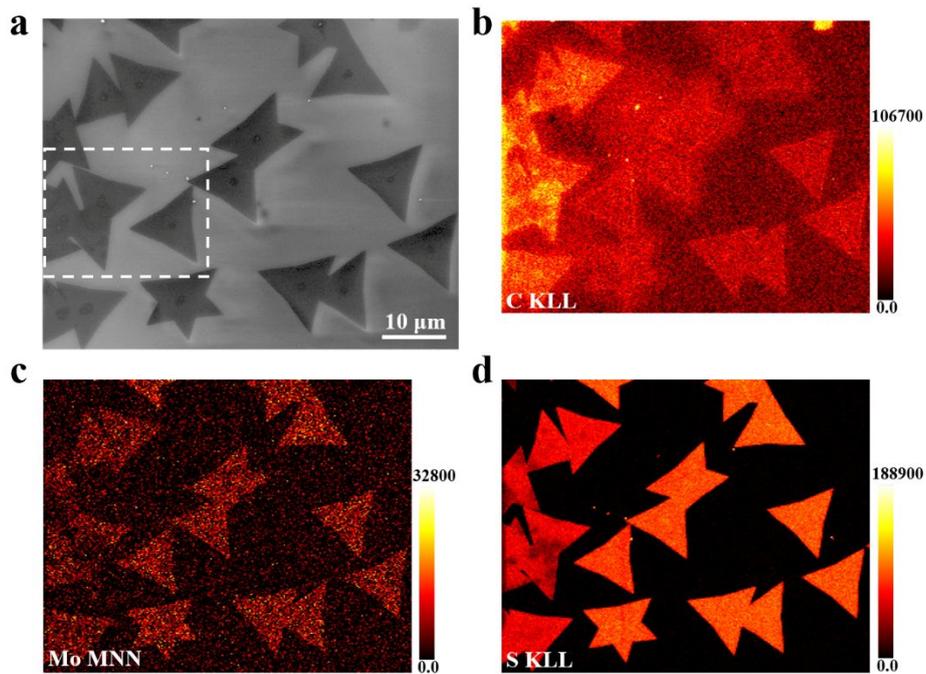


Figure S3. AES characterization of the carbon doped monolayer MoS₂ sample in a large field-view. (a) A secondary electron image of the sample showing the position for the AES elements mapping. The dash line square labels the test region shown in Figure 5. (b-d) C KLL, Mo MNN, and S KLL Auger electron element mappings of the area as (a).

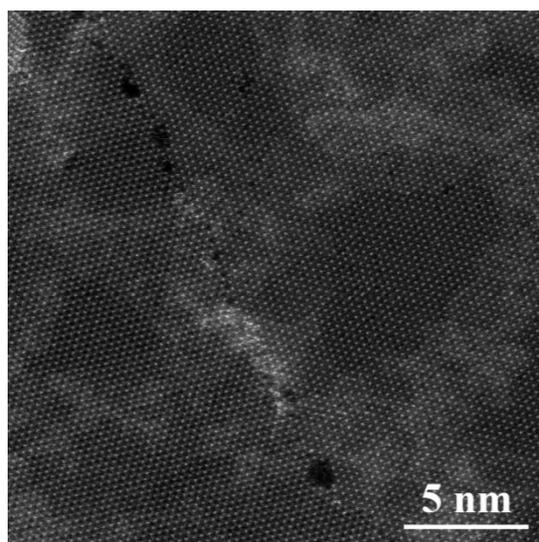


Figure S4. A STEM image of the grain boundary region of merged carbon doped MoS₂ domains showing the diverse kinds of defects.

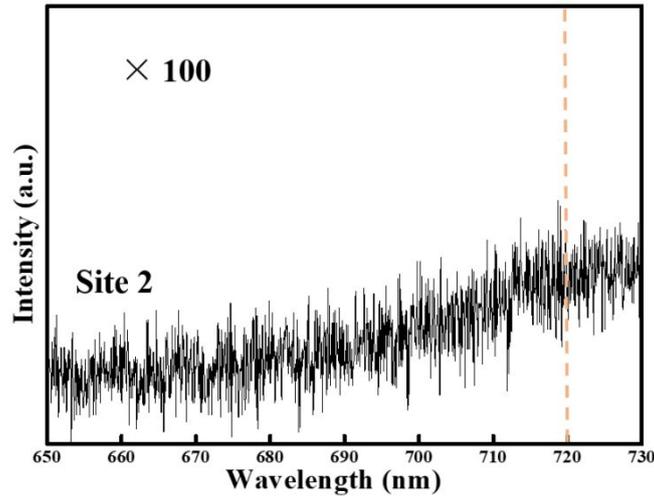


Figure S5. A 100-fold enlarged PL spectrum at site ‘2’ for Figure 5g.

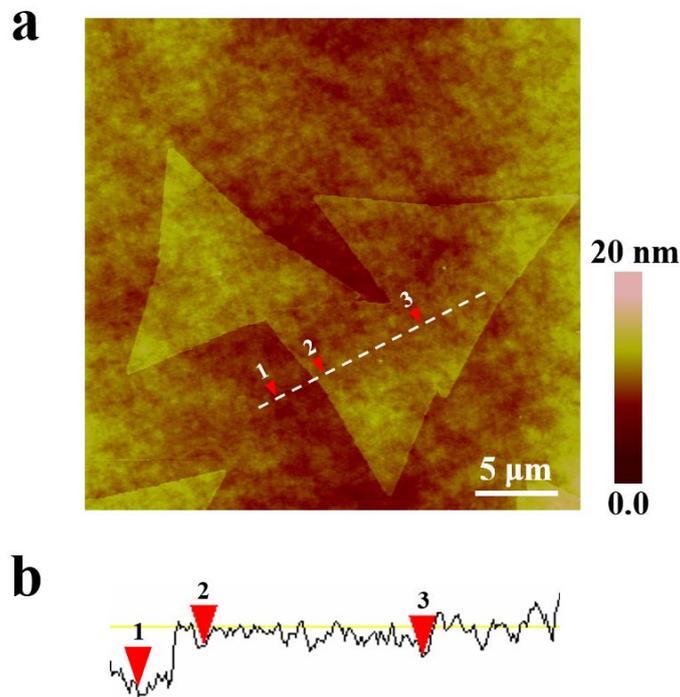


Figure S6. AFM characterization of the merging monolayer carbon-doped MoS₂ domains. (a) An AFM height image of the merging domains. (b) The height profile line along the dashed line in (a). The height distance of ~ 0.7 nm between point “1” and “2” shows the monolayer nature of the carbon-doped MoS₂ domain, and no obvious height difference is observed between point “2” and “3”, demonstrating that the domains merge in-plane without the formation of

overlapping regions.