A Metastable Pentagonal 2D Material Synthesized by Symmetry-Driven Epitaxy

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Abstract

Most 2D materials experimentally studied so far have hexagons as their building blocks[1]. Only a few exceptions, such as $PdSe_2$, are lower in energy in pentagonal phases and exhibit pentagons as the building blocks[2]. Such pentagonal 2D materials demonstrate unprecedented properties and unique applications originated from low-symmetry lattice geometries[3]. While theory has predicted a large number of pentagonal 2D materials, many of them are metastable and their experimental realization is difficult[3]. Here, we report the first successful synthesis of a metastable pentagonal 2D material, the pentagonal $PdTe_2$ monolayer, by symmetry-driven epitaxy. Scanning tunneling microscopy and complementary spectroscopy measurements are used to characterize the monolayer pentagonal $PdTe_2$, which demonstrates well-ordered low-symmetry atomic arrangements and is stabilized by lattice-match with the underlying Pd(100) substrate. In contrast, the more common hexagonal $PdTe_2$ can be grown on Pd(111). Theoretical calculations, along with angle-resolved photoemission spectroscopy, reveal the band structures of monolayer pentagonal $PdTe_2$. In contrast to the narrow bandgap of monolayer hexagonal $PdTe_2$, monolayer pentagonal $PdTe_2$ is a semiconductor with a much bigger indirect bandgap of 1.08 eV. Our work opens an avenue for the synthesis of new, pentagon-based 2D materials and gives great opportunities to explore their applications such as multifunctional electronics.

References

[1] Novoselov, K. S., Mishchenko, A., Carvalho, A. & Castro Neto, A. H. Science 353 (2016) aac9439
[2] Oyedele, A. D. et al. J. Am. Chem. Soc. 139 (2017) 14090-14097
[3] Shen, Y. & Wang, Q. Phys. Rep. 964 (2022) 1-42

Figures

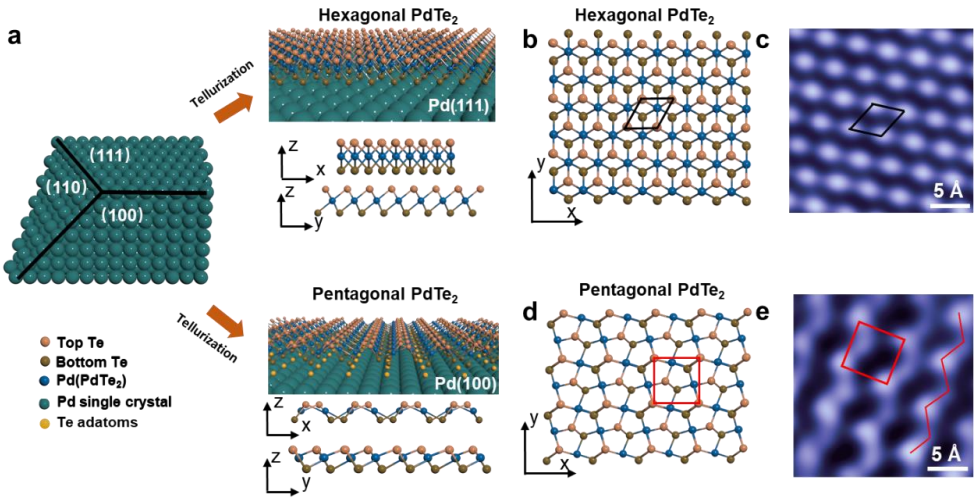

Figure 1: Synthesis of monolayer hexagonal and pentagonal $PdTe_2$.