

Abstract Submitted  
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**Morphology control of WS<sub>2</sub> monolayer islands: triangles, stars, and snowflakes** YUANXI WANG, Penn State University, CHENG-ING CHIA, Duke University, ANA ELIAS, NESTOR PEREA-LOPEZ, A. C. BELTRAN, A. BERKDEMIR, Penn State University, HUMBERTO GUTIERREZ, University of Louisville, FLORENTINO LOPEZ-URIAS, HUMBERTO TERRONES, MAURICIO TERRONES, VINCENT CRESPI, Penn State University — Interfaces play an important role in determining the electronic structure and equilibrium morphologies of monolayer nanoclusters. An additional difficulty for polar materials is that a conventional edge energy calculation using a nanoribbon exposes two different types of edge terminations, making the energy of each edge inextricable. Based on density functional theory, we report the energies of different types of edge terminations of monolayer WS<sub>2</sub> at different experimental environments in terms of varying chemical potentials of the W and S species. The Wulff construction is then applied to show that triangular shapes are most favorable at higher S chemical potential, where bulk sulfur start to become present in the system. Our results are in agreement with recent experiments that triangular islands of WS<sub>2</sub> are synthesized by CVD method using vaporized sulfur. Stacking energetics and kinetic growth factors will also be discussed to explain the formation of six-pointed star shapes and edge irregularities.

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