

# PdSe<sub>2</sub> Single Crystals Synthesized by Flux Method

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PdSe<sub>2</sub> possesses a low-symmetry pentagonal, layered structure. With unique atomic arrangement leads to interesting mechanical properties, including unusual negative Poisson's ratio and ultra-high mechanical strength [1]. Furthermore, this low-symmetry structure offers new characteristics for in-plane anisotropy in optics and electronics. For example, PdSe<sub>2</sub> possesses a strong linear dichroism ratio, up to 1.9, which can act as a high polarization-sensitive photodetector [2]. Notably, both chemical vapor deposition (CVD) grown and exfoliated PdSe<sub>2</sub> exhibit extremely high air quality stability and device performance stability, which provides an excellent opportunity for future large-scale electronic device applications. Palladium diselenide (PdSe<sub>2</sub>), a noble metal dichalcogenide, has emerged as a new 2D material with widely tunable bandgap for device applications, however the direct synthesis of high-quality PdSe<sub>2</sub> is still challenging. Here we demonstrate the growth process of single-crystal PdSe<sub>2</sub>. The PdSe<sub>2</sub> single crystal was synthesized by a self-flux (high-temperature solution) method using Se as a fluxing agent. Selenium with a purity of 99.999% was used as a solvent and a preliminary solid-phase synthesis of the compound PdSe<sub>2</sub> was carried, using Pd and Se in stoichiometric amounts as starting materials. To carry out the crystal growth process, the synthesized material was placed in quartz ampoules pumped to a vacuum of 10<sup>-5</sup> torr. The growth process was carried out for 4 days at 850°C. Under these conditions, crystals with sizes of 2-3 cm<sup>3</sup> were obtained and crystal quality characterized by XRS, XPS and Raman spectroscopy.

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## References:

- [1] Lei, W.; Cai, B.; Zhou, H.; Heymann, G.; Tang, X.; Zhang, S.; Ming, X. Ferroelastic lattice rotation and band-gap engineering in quasi 2D layered-structure PdSe<sub>2</sub> under uniaxial stress. *Nanoscale* 2019, 11, 12317–1232
- [2] Zhang, G.; Amani, M.; Chaturvedi, A.; Tan, C.; Bullock, J.; Song, X.; Kim, H.; Lien, D.-H.; Scott, M.C.; Zhang, H.; et al. Optical and electrical properties of two-dimensional palladium diselenide. *Appl. Phys. Lett.* 2019, 114, 253102

