Liangbo Liang
Kai Xiao, Alexander A. Puretzky, Giang Nguyen, An-Ping Li, David B. Geohegan, Bobby G. Sumpter
Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831
liangl1@ornl.gov

$PdSe_2$: a Pentagonal Layered Material Bridging the Gap Between 2D and 3D Materials

$PdSe_2$ is a new layered material with an in-plane pentagonal network and stronger-than-vdW interlayer coupling. It offers great trade-off between carrier mobility, band gap, and air stability for nanoelectronics [1]. Because of its unique atomic structure and strong interlayer coupling, it behaves like 2.5D material and many of its properties are different from those of commonly known 2D materials, such as graphene and MoS_2. Here I will highlight how first-principles modeling/simulation guided experiments to explore its structural, electronic, and vibrational properties. Because of strong interlayer coupling, its electronic band gap varies significantly from 1.3 eV (monolayer) to 0.06 eV (bulk), based on calculations and measurements [1]. For 2D graphene and MoS_2 that have weak interlayer interactions, the layers are quasi-rigid in low-frequency interlayer vibrations, which can be described by a linear chain model (LCM); however, in $PdSe_2$ the layers are no longer quasi-rigid, according to our Raman scattering calculations and measurements. Therefore, the thickness dependence of the interlayer Raman modes' frequencies in $PdSe_2$ deviates significantly from the LCM. A revised LCM was developed to account for the layer non-rigidity [2]. Finally, according to our nudged elastic band calculations, the pentagonal structure and strong interlayer coupling lead to low diffusion barriers for defects, and hence both intralayer and interlayer hopping of defects can occur relatively easily in $PdSe_2$ compared to MoS_2, as observed by scanning tunneling microscope [3]. Our works on $PdSe_2$ pave the road for the understanding of 2D materials featuring strong and beyond-vdW interlayer interactions.

References

[1] A. Oyedele*, S. Yang*, **L. Liang***, A. Puretzky, P. Yu, P. Pudasaini, Z. Liu, B. Sumpter, M. Chisholm, W. Zhou, P. Rack, D. Geohegan, K. Xiao, *Journal of the American Chemical Society*, 139 (2017), 14090. [*Co-lead author]
[2] A. Puretzky*, A. Oyedele, K. Xiao, B. Sumpter, D. Mandrus, D. Geohegan, **L. Liang***, *2D Materials*, 5 (2018), 035016. [*Corresponding author]
[3] G. Nguyen, **L. Liang***, Q. Zou, M. Fu, A. Oyedele, B. Sumpter, Z. Liu, Z. Gai, K. Xiao, A. Li*, *Physical Review Letters*, 121 (2018), 086101. [*Corresponding author]

Figures

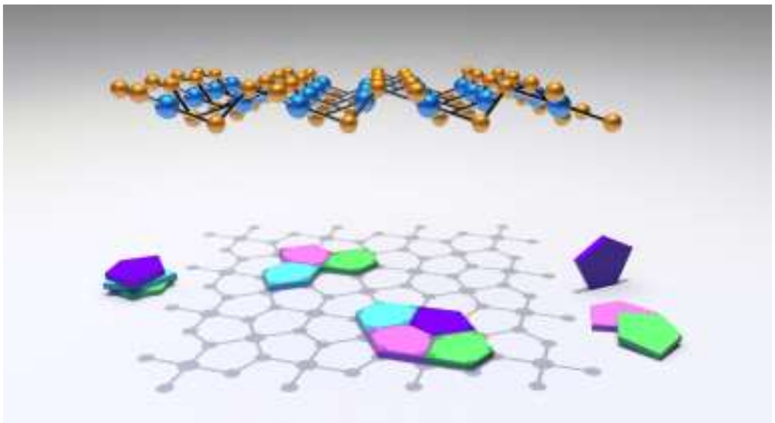

Figure 1: $PdSe_2$, a novel layered material with atoms that tile in the famous Cairo pentagonal pattern. It behaves like a 2.5D material due to the unique atomic structure and stronger-than-vdW interlayer coupling.

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