Effects of Electromechanical Coupling in Locally Strained Monolayer MoS_2

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Strain in atomically thin transition metal dichalcogenides (TMDs) has a broad range of consequences, and can be used for tuning of their optical and electronic properties [1, 2]. In particular, the use of localized strain to engineer these effects, such as in exciton funneling, has been demonstrated [3]. Additionally, TMDs exhibit intrinsic piezoelectricity in monolayer and few layer form originating from a lack of centrosymmetry [4]. The presence of piezoelectricity in TMD systems with strain and strain gradients can also have appreciable effects, which have only begun to be explored. Understanding these effects is necessary for engineering of TMD-based structures in which strain is present.

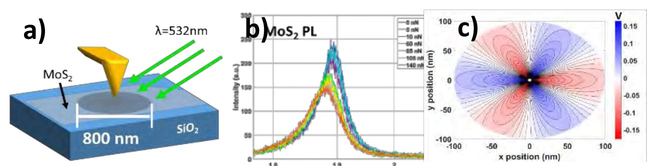

Figure 1: (a) Schematic depicting indentation and PL characterization. (b) PL measurement of MoS_2 during indentation. (c) Calculated electrostatic potential from piezoelectricity in indented MoS2

In this work, we examine the effects of piezoelectricity on MoS_2 in the presence of strain and strain gradients. Samples consisting of monolayer MoS2 suspended over 800nm-diameter cavities were fabricated by exfoliation and transfer of MoS_2 onto a patterned substrate. Suspended MoS_2 was deformed via atomic force microscope (AFM) indentation, and Photoluminescence (PL) measurements were simultaneously performed as a function of indentation force to determine the effects of the strain gradient on exciton bandgap and exciton diffusion (Fig. 1a, b). Additionally, we show through calculations that spatially varying strain, can be a source of electrostatic potentials due to the piezoelectric effect. According to a mechanical model for indentation [5], the charge density can be as high as 10^{12} e/cm^2 at the points of highest strain gradient - significant enough to generate electrostatic potential variations on the order of ±0.1V over the MoS_2 (Fig. 1c). The relationship between strain and the potential generated by piezoelectricity, and the impact of this effect on excitons, will be discussed.

[1] H. Conley, B. Wang, J. Ziegler, R. Haglund Jr., S. Pantelides, K. Bolotin, Nano Lett. 12, 8 (2013)
[2] T. Shen, A. V. Penumatcha, and J. Appenzeller, ACS Nano **10**, 4, 4712-4718 (2016).
[3] A. Castellanos-Gomez, R. Roldán, E. Cappelluti, M. Buscema, F. Guinea, H. S. J. van der Zant, and G. A. Steele, Nano Lett. **13**, 11, 5361-5366 (2013).
[4] Duerloo, K. A. N., Ong, M. T. & Reed, E. J., *J. Phys. Chem. Lett.* **3,** 2871–2876 (2012).
[5] N. M. Bhatia, W. Nachbar, Int. J. Non-Linear Mechanics, **3,** 307-324 (1968).

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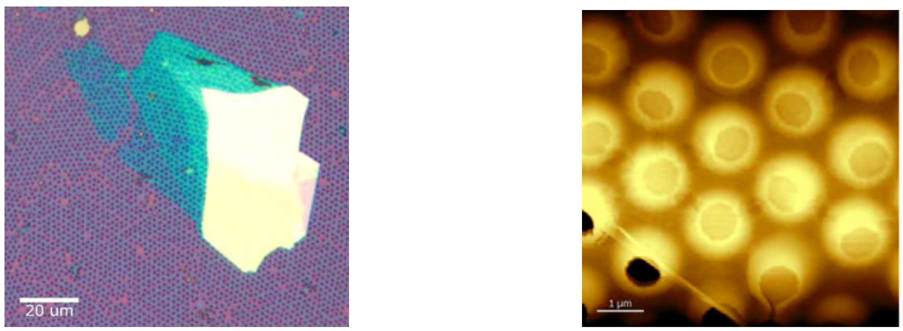

Figure S1. a) Optical image and b) AFM image of exfoliated MoS_2 transferred onto SiO_2 substrate with nanopatterned holes.

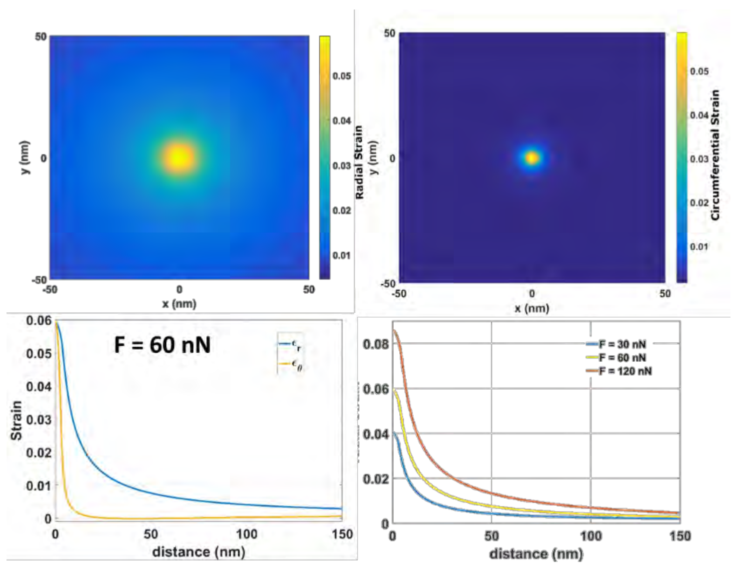

Figure S2. Calculation of the strain distribution of a circular membrane of 500nm diameter MoS_2 indented by a spherical indenter of radius 7nm. The top panels are contour plots of the distribution of a) radial and b) circumferential strain for 60 nN of indentation force. The majority of strain is confined to a very small area near the point of indentation. Profiles of the contour plots along the x-axis are shown in c), while d) shows the dependence of the strain on indentation force.

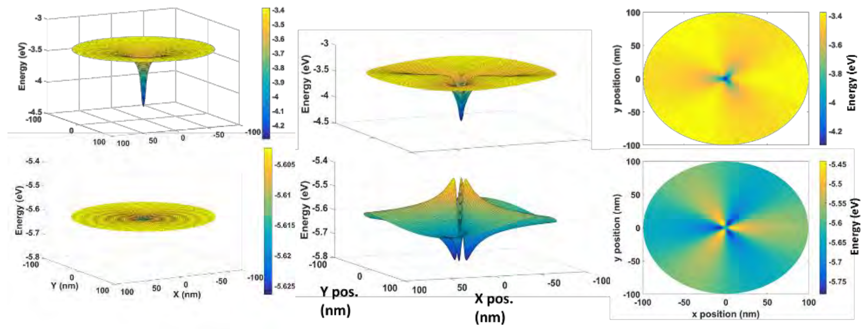

Figure S3. Analysis of the spatial distribution of the band edge at the k-point for MoS2. a) and b) depict the CBM and VBM, respectively, due to effects of strain without considering effects of piezoelectricity. The bandgap decreases towards the point of highest tensile strain. c) and d) show the same CBM and VBM distribution, only now including the effects of the electrostatic potential generated by the piezoelectric effect. From e) and f), which depict the top-down view of c) and d), it can be seen that towards the center, the minimum of the CBM does not spatially align with the maximum of the VBM.