# Electronic properties of transition metal dichalcogenide nanowrinkles and nanobubbles

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Mechanical deformations in transition metal dichalcogenide monolayers can appear both spontaneously and artificially, giving rise to structures such as nanowrinkles [1] or nanobubbles [2]. Such deformations have been observed to harbor localized exciton states, a known prerequisite for single-photon emission, triggering theoretical studies attempting to explain these phenomena. However, fully quantum-mechanical insight given by ab initio calculations is still missing to date.

We model one-dimensional MoSe2 nanowrinkles by applying uniaxial compressive strain with increasing magnitude in the plane of the monolayer [3]. We analyze their structural properties, highlighting the coexistence of local domains of tensile and compressive strain in the same system. We find that the electronic properties are driven by the curvature rather than strain; band gaps vary moderately in size compared to flat counterparts and remain direct. We finally discuss transport properties through the inspection of effective masses and identify their correlation with the localization of wave-function distributions.

Additionally, we create two-dimensional MoS2 nanobubbles using two types of deformation-inducing forces, labeled as "uniform" and "central" load [4]. We observe a reduction in the band gap accompanied by a direct-to-indirect transition for both types of defects. We also identify intervalley scattering in the conduction band, which is conjectured to be the enabling factor behind single-photon emission. We further examine the effect of single S atom vacancies, which are commonly encountered in practice. These vacancies result in additional localized gap states, with their depth varying with the exact site of the vacancy.

The identification of localized states in both nanowrinkles and nanobubbles provides valuable insight into the microscopic origins of optoelectronic features. This emphasizes the promising potential of these systems as active components for (opto)electronic devices.

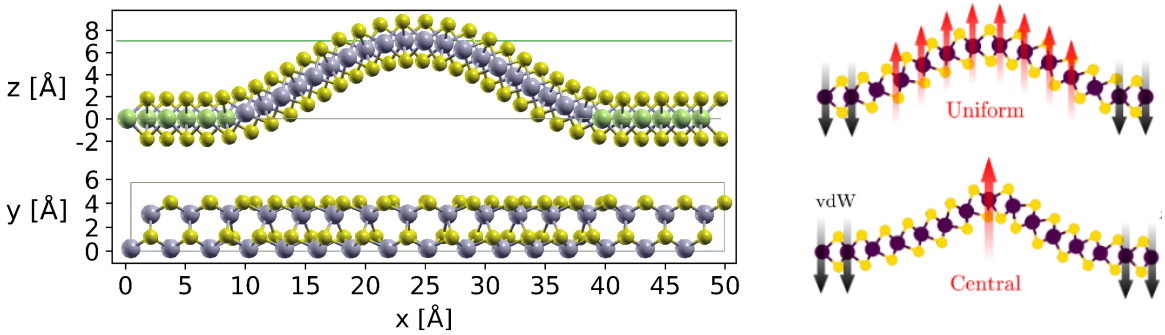


Figure: An example $MoSe_2$ nanowrinkle, seen from the side and above (left panel). An illustration of the $MoS_2$ nanobubble, highlighting the uniform and central forces inducing the deformation (right panel).

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[2] G. D. Shepard, O. A. Ajayi, X. Li, X. Y. Zhu, J. Hone, S. Strauf, 2D Mater. 2017, **4**, 2, 021019.
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