Effect of mechanical deformations in electronic properties of transition metal dichalcogenides

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Transition-metal dichalcogenides (TMDs) have recently attracted a great interest, particularly in their 2D monolayer forms, following comprehensive research on graphene. Despite the outstanding electrical properties of graphene, its application in nanoelectronic and nanophotonic devices is restricted due to zero band gap. The semiconducting TMD monolayers with extraordinary properties, such as distinct band gap, high carrier mobility and high thermal stability, are expected to have a promising potential in future nanoelectrodevices. Similar to graphene, 2D TMDs can be produced from their bulk material through liquid phase exfoliation process. Recently, these novel 2D systems have been used to fabricate first field-effect transistors, logical circuits and amplifiers [1,2].

We have found that the electronic structure of layered TMDs can be tuned by different strategies, such as quantum confinement, nanotube formation, substitutional doping or mechanical deformations [3-5]. In this work, electronic properties of TMD monolayers are studied as subject to mechanical deformations, namely strain and rippling. Under 2D-isotropic strain, the TMD monolayers change the semiconducting direct-gap character and become metallic for the deformations as large as 11%, what results in electrical conductivity at the Fermi level. On the other hand, the formation of ripples causes extreme quenching of the conductance. In addition, we have studied strain effects on the electronic and transport characteristics of TMD nanotubes.

References

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