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Mechanical Stability and Elastic Properties of Monolayer SnS_2: A First-Principles Study

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Abstract
In this work, we report on a thorough first principles study of the mechanical stability and in plane elastic properties of monolayer SnS_2 within the DFT framework. We used the finite strain approach for evaluation of the elastic response which included application of small uniaxial, biaxial and shear deformations (of up to ±0.5% and ±1%) to the fully relaxed structure. We found that the strain energy relationships which resulted are very well defined and quadratic in nature which in turn confirms that our applied deformations are within the harmonic elastic regime. In our study, we used second order polynomial fitting of the strain which in turn gave us the independent in plane elastic constants of C_{11} = 81.4 N/m, C_{12} = 9.2 N/m, and C_{66} = 14.1 N/m. Also we determined the shear modulus from the curvature of the shear strain – energy plot without imposing any symmetry constraints. We found that the 2D Young's modulus which we got is about 80.3 N/m and Poisson's ratio at around 0.113 which indicates a material that has moderate in plane stiffness and also sees relatively large transverse strain. We find that the elastic constants we have obtained do in fact meet the Born mechanical stability criteria which in turn confirms the very intrinsic mechanical robustness of monolayer SnS_2. Also we see that the shear modulus is relatively low when compared to the longitudinal stiffness which may point to an anisotropic elastic response within the calculated accuracy. We present here a solid theoretical base for strain engineering and also for the use of SnS_2 monolayers in flexible nanoelectronics.
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I. Introduction

In the past two-dimensional (2D) materials have transformed the fields of condensed matter physics and materials science which is a result of their remarkable electronic, optical, and mechanical properties that come about from atomic scale confinement[1-3]. Out of the successful isolation of graphene we have seen the emergence of layered transition metal dichalcogenides (TMDs) which have become a very versatile class of 2D semiconductors with tune able band structures, strong light-matter interactions and very promising for device applications[4-6]. Also what we see in TMDs is a great structural diversity and low dimensionality which makes them very attractive for the development of next generation nanoelectronic, optoelectronic and energy related technologies[7, 8].

In the TMD family Tin disulfide (SnS_2) has gained much attention recently for its abundance in the earth, chemical stability, and also because of its benign environmental profile[9-11]. SnS_2 has a CdI_2-type layered hexagonal structure which is made up of S – Sn – S sandwiches that are stacked via weak van der Waals forces[12, 13]. Upon being exfoliated to the monolayer scale we see modified electronic and optical properties which is a result of quantum confinement and reduced interlayer coupling which in turn makes it a great fit for use in photodetectors, sensors and energy storage systems[1, 14, 15].

Although, we have a very good handle on the electronic structure of SnS_2 what we don't know as much about is its mechanical behavior[16, 17]. Mechanical stability and elastic properties are very important in the practical use of 2D materials in flexible electronics, strain engineered devices, and in the design of heterostructures[18-20]. At the atomic scale in these very thin materials even small changes in the lattice structure can greatly affect electronic states, carrier mobility and optical transitions[21, 22]. Thus we require an in depth knowledge of elastic constants and mechanical stability which is key to predict device reliability and tolerance to strain[23, 24].

In terms of theory Density Functional Theory (DFT) is a reliable base we use to study the elastic response of low dimensional materials with finite strain methods[25-27]. We apply controlled lattice deformations and look at the strain – energy relationship to determine the independent elastic constants in the harmonic approximation[28, 29]. From there we determine key mechanical parameters like Young's modulus, Poisson's ratio, and shear modulus which in turn tell us about the material's stiffness, transverse coupling, and resistance to shear[30, 31].

In our work, we report a detailed first principles study of the in plane elastic properties of monolayer SnS_2. We apply finite strain approach to which we subject the fully relaxed structure to small uniaxial, biaxial and shear deformations and from there we analyze the strain – energy relationships to determine the independent elastic constants. We also very rigorously assess mechanical stability through the Born criteria for 2D systems. What we find is that we gain into the intrinsic stiffness and deformation behavior of monolayer SnS_2 in detail and at the same time we set a very consistent theoretical base for what is to come in terms of strain engineering and flexible device applications.

II. Computational Methodology

2.1 First-Principles Calculations

In the present study, we used Density Functional Theory (DFT) within the Quantum ESPRESSO package for all our calculations[32]. We used the Generalized Gradient Approximation (GGA) in its Perdew – Burke – Ernzerhof (PBE) formulation to account for exchange – correlation interaction[33]. Also we applied norm conserving pseudopotentials which we used to describe ion – electron interactions[34, 35]. In our study, we used a plane wave kinetic energy cutoff of 40 Ry for the wave functions, also we set the charge density cutoff at 320 Ry. For the Brillouin zone we used a 4 x 4 x 1 Monkhorst – Pack k point mesh. Also to remove artificial interaction between periodic layers in the out of plane direction we introduced a vacuum spacing of about 23 Å.

In our work, we fully optimized atomic positions using the Broyden – Fletcher – Goldfarb – Shanno (BFGS) algorithm which we continued until we achieved a residual force of less than 10^{-3} Ry/Bohr on each atom and also a total energy convergence better than 10^{-4} Ry. That optimized structure we used as a reference for all of our subsequent elastic property calculations.

2.2 Elastic Constant Calculation

In plane elastic constants we determined using the finite strain method within the harmonic approximation[36, 37]. We applied lattice deformations of ±0.5% and ±1% to the fully optimized monolayer structure which we did so in three independent deformation mode:

- Uniaxial strain (εx)
- Biaxial strain ($\varepsilon x = \varepsilon y$)
- In-plane shear strain (γ)

For each applied strain we saw that the lattice vectors changed as they should while the internal atomic coordinates had free rein to relax within the strained cell. We calculated the total energy for each deformation and also did a second order polynomial fit to the strain dependent energy variation[38].

$E(\varepsilon) = E_0 + A\,\varepsilon^2 + B\,\varepsilon$

where E_0 is the equilibrium total energy and ε is the strain parameter.

The linear term was found to be negligible ($B \approx 0$), consistent with symmetric deformation about zero strain.

In order to get the 2D elastic constants we normalized energy differences by the equilibrium in plane area (A_0) which in turn gave us the strain energy density[26]:

$U(\varepsilon) = \Delta E / A_0$

We determined the quadratic fit which in turn we used to extract the related elastic constants. In particular, the shear modulus (C_{66}) was obtained by us from the curvature of the shear strain energy relation which we did not impose to conform to symmetry. This full numerical approach we found to accurately determine the independent in plane elastic constants within the harmonic deformation regime.

III. Elastic Theory for Two-Dimensional Systems

3.1 Strain Energy Formalism

For a 2D crystal under small deformations the strain energy density within a harmonic approximation is represented by a quadratic function of the strain tensor components[25]. In Voigt notation we write the in plane strain components as:

$\varepsilon_1 = \varepsilon xx$, $\varepsilon_2 = \varepsilon yy$, $\varepsilon_6 = \gamma xy$

where, γxy denotes the in-plane engineering shear strain.

The elastic strain energy density per unit area can be written as:

$U = \frac{1}{2} C_{11}\, \varepsilon_1^2 + \frac{1}{2} C_{22}\, \varepsilon_2^2 + C_{12}\, \varepsilon_1 \varepsilon_2 + \frac{1}{2} C_{66}\, \varepsilon_6^2$

For systems with in-plane symmetry equivalent along x and y directions ($C_{11} = C_{22}$), this expression simplifies to:

$U = \frac{1}{2} C_{11} (\varepsilon x^2 + \varepsilon y^2) + C_{12}\, \varepsilon x\, \varepsilon y + \frac{1}{2} C_{66}\, \gamma^2$

This model which we present is the foundation for the determination of elastic constants from strain energy relationships which in turn we obtain via first principles calculations.

3.2 Determination of Elastic Constants

Under uniaxial strain ($\varepsilon x \neq 0$, $\varepsilon y = 0$, $\gamma = 0$), the strain energy density reduces to:

$U = \frac{1}{2} C_{11}\, \varepsilon x^2$

Under biaxial strain ($\varepsilon x = \varepsilon y = \varepsilon$, $\gamma = 0$), the energy expression becomes:

$U = (C_{11} + C_{12})\ \varepsilon^2$

For pure shear deformation ($\gamma \neq 0$, $\varepsilon x = \varepsilon y = 0$), the energy density is:

$U = ½\ C_{66}\ \gamma^2$

Thus, by fitting the strain-dependent energy density to a second-order polynomial:

$U(\varepsilon) = a\ \varepsilon^2$

the elastic constants can be directly extracted from the curvature coefficients of the corresponding strain modes.

3.3 Mechanical Stability Criteria

Mechanical stability of a two-dimensional crystal requires that the elastic strain energy remains positive for any small arbitrary deformation[2]. This condition leads to the Born stability criteria:

$C_{11} > 0$, $C_{66} > 0$, $C_{11} - C_{12} > 0$

Satisfaction of these inequalities ensures that the system is mechanically stable within the harmonic deformation regime.

3.4 Derived Mechanical Parameters

From the independent elastic constants, additional mechanical properties can be derived. The in-plane Young's modulus (Y) and Poisson's ratio (ν) are given by:

$Y = (C_{11}^2 - C_{12}^2) / C_{11}$, $\nu = C_{12} / C_{11}$

These parameters define the axial stiffness and transverse strain response of the material which in turn gives a full picture of it's in plane mechanical behavior.

IV. Results and Discussion

4.1 Structural Stability and Equilibrium Geometry

In Figure 1 we present the optimized atomic structure for monolayer SnS_2. Also we see that the fully relaxed geometry which preserves the hexagonal symmetry of the CdI_2-type layered structure. In Figure 1(a) we see the top view which shows the in plane hexagonal arrangement of Sn and S atoms; here tin atoms form a triangular lattice that is symmetrically surrounded by sulfur atoms. In Figure 1(b) we can see that the side view clearly shows the characteristic S – Sn – S trilayer structure in which a single tin layer is trapped between two of sulfur's. In Figure 1(c) we present the atomic configuration under in plane shear strain. In the applied deformation the simulation cell transforms into a parallelogram geometry which at the same time preserves the S – Sn – S bonding framework that which says the structure of the mon layer does in fact remain intact within the harmonic elastic regime. We note that there is no structural instability or bond breaking which in turn confirms the mechanical robustness of our optimized structure and we use it as the reference configuration for further elastic calculations.

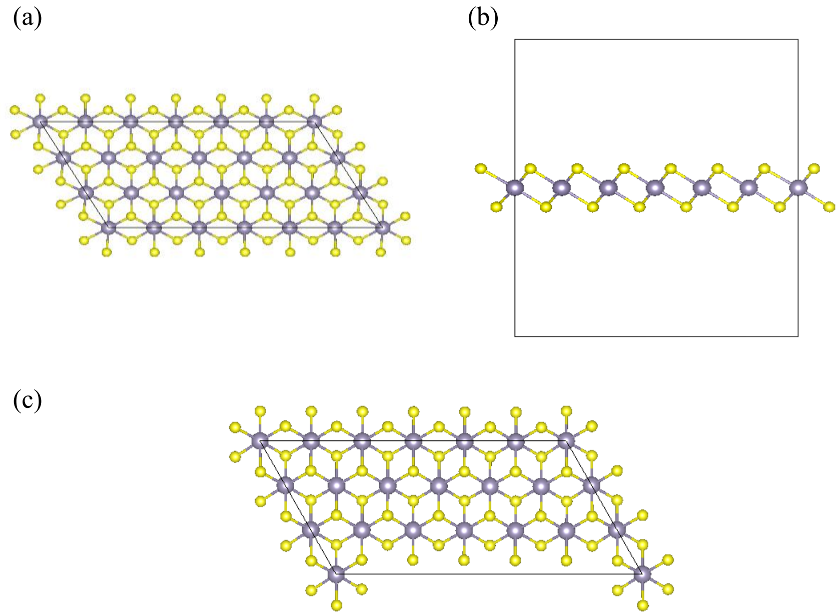

Figure 1. Optimized and shear deformed atomic structures of monolayer SnS_2. (a) Top view of the relaxed hexagonal lattice; (b) Side view showing the S–Sn–S trilayer configuration;(c) Structure under in-plane shear strain illustrating the elastic deformation of the simulation cell.

4.2 Strain–Energy Relationship

In order to assess the elastic response, we applied small in plane deformations in uniaxial, biaxial and shear strain conditions. We calculated the strain energy density by which we divided the total energy change by the equilibrium in plane area. In Figure 2 we present the strain energy relationship under uniaxial deformation. We see that energy variation displays a very definite quadratic trend in strain, also we note almost identical response under tensile and compressive loading which in turn confirms that our applied deformation is within the harmonic elastic range.

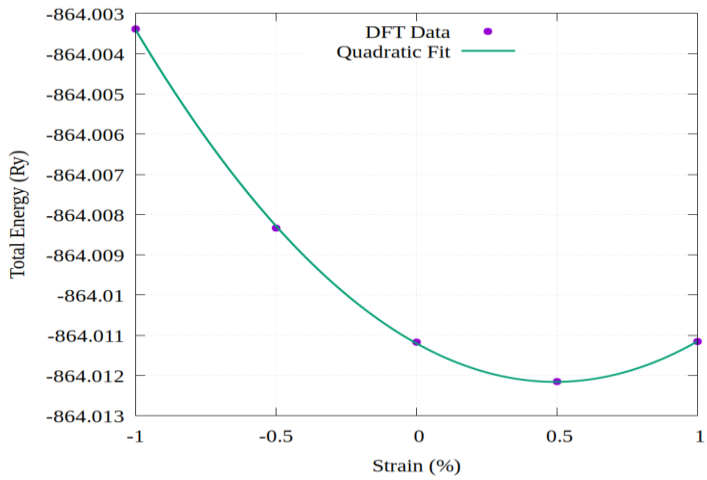

Figure 2. Strain energy density as a function of uniaxial strain (εx) for monolayer SnS_2. The quadratic fitting confirms harmonic elastic behavior.

Also we see in Figure 3 that the biaxial strain energy relationship has a very clear quadratic trend. Zero strain symmetry which we note is present in the graph is an indicator of numerical consistency and stable elastic behavior under uniform in plane deformation.

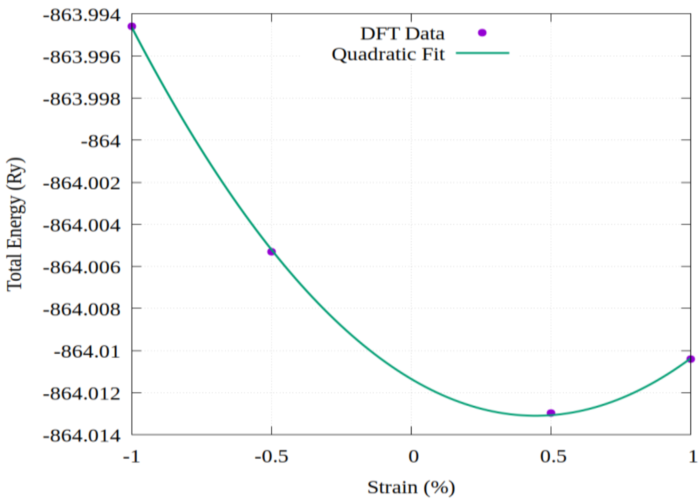

Figure 3. Strain energy density versus biaxial strain (εx = εy) for monolayer SnS_2

4.3 Shear Deformation and Shear Modulus

In figure 4, we present the in plane shear response of monolayer SnS_2. Upon application of shear strain the simulation cell transforms into a parallelogram shape, yet the structure of the S–Sn–S framework remains intact. In our experiments we observed a quadratic relationship between strain and energy at low shear strains which we used to determine the shear modulus C_{66}. Also we found that structure preservation under shearing confirms the applied strain is within the elastic range.

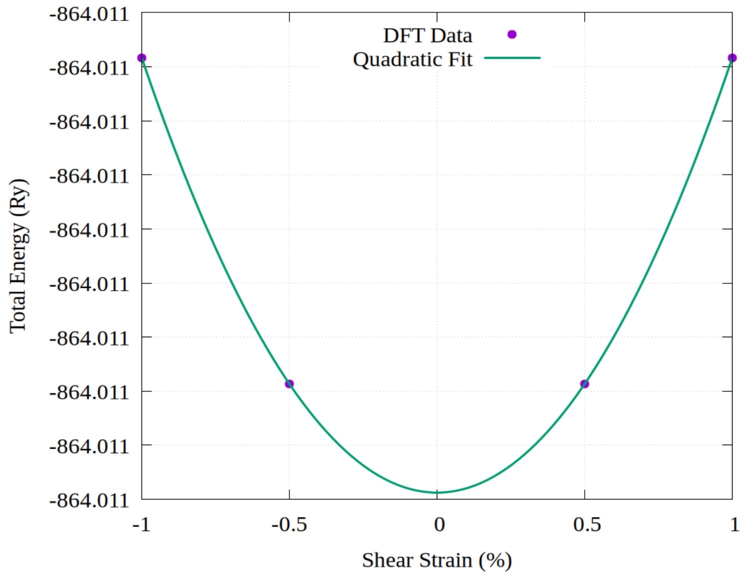

Figure 4. Strain energy density as a function of in-plane shear strain (γ) for monolayer SnS_2. The curvature of the quadratic fit was used to determine the shear modulus C_{66}.

4.4 In-Plane Elastic Constants
From our analysis of the strain energy density under uniaxial, biaxial, and shear deformations, see Figures (2 – 4) we determined the independent in plane elastic constants for monolayer SnS_2 which:

$$C_{11} = 81.4 \text{ N/m}$$
$$C_{12} = 9.2 \text{ N/m}$$
$$C_{66} = 14.1 \text{N/m}$$

In this case C_{11} is the longitudinal in plane stiffness which also includes the term for the transverse elastic coupling between orthogonal directions. Also we have C_{66} which we obtain from the curvature of the shear strain energy curve without having to apply symmetry relations it is a measure of the lattice's resistance to angular deformation.

From these elastic constants we have determined the values of the 2D Young's modulus and Poisson's ratio which are:

$$Y \approx 80.3 \text{ N/m}$$
$$\nu \approx 0.113$$

In terms of Young's modulus, we see a moderate in plane stiffness, also the low Poisson's ratio reports which there is little lateral contraction during tensile loading which is a character of the layer bonded structure of SnS_2.

4.5 Mechanical Stability and Anisotropy
We find that the calculated elastic constants meet the Born mechanical stability criteria for a 2D system:

$$C_{11} > 0$$
$$C_{66} > 0$$
$$C_{11} - C_{12} > 0$$

Reporting that we see in the harmonic deformation regime the inherent mechanical stability of SnS_2. To assess in plane elastic an isotropy the an isotropy factor was determined as:

$$A = 2C_{66}/(C_{11} - C_{12})$$

We see that $A \sim 0.39$. In a perfect 2D isotropic system $A = 1$, which we do not see here instead we see an anisotropic shear response. It is true that the shear strain energy diagram does play out perfectly symmetrically around zero strain which in turn demonstrates numerical consistency and that we have pure harmonic elastic behavior. That said this symmetry what it does is reflect elastic stability as opposed to perfect mechanical isotropy. Also we see that the shear curve has a lesser degree of curvature as compared to the uniaxial case which in turn is a sign of the monolayer's lower resistance to shear deformation.

V. Conclusion

In this work, we report a thorough first principles study of the in plane elastic properties of monolayer SnS_2 within the density functional theory framework. We found that the optimized structure which preserves the hexagonal CdI_2-type symmetry serves as a very reliable reference for our mechanical analysis.

In the range of ±1% strain we see a clear quadratic trend in the strain energy for uniaxial, biaxial and shear deformations which in turn confirms that the system is in the harmonic elastic regime. Also we report that the extracted elastic constants (C_{11} = 81.4 N/m, C_{12} = 9.2 N/m and C_{66} = 14.1 N/m) meet the Born mechanical stability criteria which in turn proves the intrinsic mechanical stability of the monolayer.

In our study, we report a Young′s modulus (Y ≈ 80.3 N/m) which we note as average but not high in the group of 2D materials, at the same time the Poisson ratio which we see at (ν ≈ 0.113) is quite low that which in turn means that the material doesn't contract laterally as much as it does in other materials under tens also we note that the lowered shear rigidity is a true indication of a very flexible lattice structure.

In general, mechanical robustness in conjunction with elastic flexibility has been found in monolayer SnS_2 which in turn makes it a very good candidate for use in flexible nanoelectronic systems and strain engineered devices. Also our results present a quantified mechanical base which will serve as a background for going forward in both experimental and theoretical study of SnS_2 based 2D heterostructures and functional materials.

References

[1]. Chang, C., et al., Recent progress on two-dimensional materials. Wuli Huaxue Xuebao/Acta Physico-Chimica Sinica, 2021.

[2]. Kim, J.H., et al., Mechanical properties of two-dimensional materials and their applications. Journal of Physics D: Applied Physics, 2019. **52**(8): p. 083001.

[3]. Xu, M., et al., Graphene-like two-dimensional materials. Chemical reviews, 2013. **113**(5): p. 3766–3798.

[4]. Tao, L., et al., Enhancing light-matter interaction in 2D materials by optical micro/nano architectures for high-performance optoelectronic devices. InfoMat, 2021. **3**(1): p. 36–60.

[5]. Huang, L., et al., Enhanced light–matter interaction in two-dimensional transition metal dichalcogenides. Reports on Progress in Physics, 2022. **85**(4): p. 046401.

[6]. Li, Z.-W., et al., Light–matter interaction of 2D materials: Physics and device applications. Chinese Physics B, 2017. **26**(3): p. 036802.

[7]. Chowdhury, T., E.C. Sadler, and T.J. Kempa, Progress and prospects in transition-metal dichalcogenide research beyond 2D. Chemical reviews, 2020. **120**(22): p. 12563–12591.

[8]. Ponraj, J.S., et al., Photonics and optoelectronics of two-dimensional materials beyond graphene. Nanotechnology, 2016. **27**(46): p. 462001.

[9]. Norton, K.J., F. Alam, and D.J. Lewis, A review of the synthesis, properties, and applications of bulk and two-dimensional tin (II) sulfide (SnS). Applied Sciences, 2021. **11**(5): p. 2062.

[10]. Rani, D., Synthesis of Tin Disulfide (SnS2) and its Characterization. 2022, HARYANA AGRICULTURAL UNIVERSITY HISAR.

[11]. Shinde, P. and C.S. Rout, Advances in synthesis, properties and emerging applications of tin sulfides and its heterostructures. Materials Chemistry Frontiers, 2021. **5**(2): p. 516–556.

[12]. Guo, X., et al., Review on the advancement of SnS 2 in photocatalysis. Journal of Materials Chemistry A, 2023. **11**(14): p. 7331–7343.

[13]. Lu, Z., et al., 2D materials based on main group element compounds: phases, synthesis, characterization, and applications. Advanced Functional Materials, 2020. **30**(40): p. 2001127.

[14]. Alzakia, F.I. and S.C. Tan, Liquid-exfoliated 2D materials for optoelectronic applications. Advanced Science, 2021. **8**(11): p. 2003864.

[15]. Verma, A., A. Rani, and B.C. Yadav, Two-dimensional layered metal oxides (2D LMOs) for next-generation electronic devices. Nanoscale Advances, 2025.

[16]. Burton, L.A., et al., Synthesis, characterization, and electronic structure of single-crystal SnS, Sn2S3, and SnS2. Chemistry of Materials, 2013. **25**(24): p. 4908–4916.

[17]. Voznyi, A., et al., Structural and electrical properties of SnS2 thin films. Materials Chemistry and Physics, 2016. **173**: p. 52–61.

[18]. Androulidakis, C., et al., Tailoring the mechanical properties of 2D materials and heterostructures. 2D Materials, 2018. **5**(3): p. 032005.

[19]. Du, J., et al., Strain engineering in 2D material-based flexible optoelectronics. Small Methods, 2021. **5**(1): p. 2000919.

[20]. Dai, Z., L. Liu, and Z. Zhang, Strain engineering of 2D materials: issues and opportunities at the interface. Advanced Materials, 2019. **31**(45): p. 1805417.

[21]. Rondinelli, J.M. and N.A. Spaldin, Structure and properties of functional oxide thin films: insights from electronic-structure calculations. Advanced materials, 2011. **23**(30): p. 3363–3381.

[22]. Heine, T., Transition metal chalcogenides: ultrathin inorganic materials with tunable

electronic properties. Accounts of chemical research, 2015. **48**(1): p. 65–72.

[23]. Root, S.E., et al., Mechanical properties of organic semiconductors for stretchable, highly flexible, and mechanically robust electronics. Chemical reviews, 2017. **117**(9): p. 6467–6499.

[24]. Harris, K.D., A.L. Elias, and H.-J. Chung, Flexible electronics under strain: a review of mechanical characterization and durability enhancement strategies. Journal of materials science, 2016. **51**(6): p. 2771–2805.

[25]. Le Page, Y. and P. Saxe, Symmetry-general least-squares extraction of elastic data for strained materials from ab initio calculations of stress. Physical Review B, 2002. **65**(10): p. 104104.

[26]. Cooper, R.C., et al., Nonlinear elastic behavior of two-dimensional molybdenum disulfide. Physical Review B—Condensed Matter and Materials Physics, 2013. **87**(3): p. 035423.

[27]. Choudhary, K., et al., Elastic properties of bulk and low-dimensional materials using van der Waals density functional. Physical review. B, 2018. **98**(1): p. 10.1103/physrevb. 98.014107.

[28]. Parrinello, M. and A. Rahman, Strain fluctuations and elastic constants. The Journal of Chemical Physics, 1982. **76**(5): p. 2662–2666.

[29]. Wielewski, E., et al., A methodology to determine the elastic moduli of crystals by matching experimental and simulated lattice strain pole figures using discrete harmonics. Acta Materialia, 2017. **126**: p. 469–480.

[30]. Chippada, U., B. Yurke, and N.A. Langrana, Simultaneous determination of Young's modulus, shear modulus, and Poisson's ratio of soft hydrogels. Journal of Materials Research, 2010. **25**(3): p. 545–555.

[31]. Ghavamian, A., M. Rahmandoust, and A. Öchsner, On the determination of the shear modulus of carbon nanotubes. Composites Part B: Engineering, 2013. **44**(1): p. 52–59.

[32]. Lejaeghere, K., et al., Reproducibility in density functional theory calculations of solids. Science, 2016. **351**(6280): p. aad3000.

[33]. Perdew, J.P., K. Burke, and Y. Wang, Generalized gradient approximation for the exchange-correlation hole of a many-electron system. Physical review B, 1996. **54**(23): p. 16533.

[34]. Willand, A., et al., Norm-conserving pseudopotentials with chemical accuracy compared to all-electron calculations. The Journal of chemical physics, 2013. **138**(10).

[35]. Trail, J. and R. Needs, Norm-conserving Hartree–Fock pseudopotentials and their asymptotic behavior. The Journal of chemical physics, 2005. **122**(1): p. 014112.

[36]. John, F., Plane strain problems for a perfectly elastic material of harmonic type. Communications on Pure and Applied Mathematics, 1960. **13**(2): p. 239–296.

[37]. Hearmon, R., The elastic constants of anisotropic materials. Reviews of modern physics, 1946. **18**(3): p. 409.

[38]. Khachaturyan, A., S. Semenovskaya, and T. Tsakalakos, Elastic strain energy of inhomogeneous solids. Physical Review B, 1995. **52**(22): p. 15909.