Predicting the strain effects in 2D materials: the case of ZrS3 monolayers

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Thermoelectric materials have attracted much attention because they produce electricity without moving parts, which makes them ideal to engineer reliable devices that require minimal maintenance for long periods for applications such as harvesting human body heat and solar generators. We present here the influence of strained deformations on the mechanical and electronic properties of ZrS3 monolayers. Density functional theory (DFT) calculations are employed at the hybrid HSE06 level on the atomistic structures optimised with PBE to evaluate the anisotropic response of the electronic band gap and mobilities, as well as the thermopower, the electrical and thermal conductivities, and the figure of merit. Direct examination of the electronic band structures reveals that the band gap can be increased by up to 17% under uniaxial strain, reaching up to 2.32 eV for ZrS3. We also detect large variations in the electrical conductivity in this material, which is multiplied by 3.40 under a 4% compression for ZrS3. In contrast, our DFT calculations predict much smaller changes in the Seebeck coefficient. In addition, the modelling of mechanical deformation is also used to find the anisotropic behaviour of the Poisson ratios. We also present at which conditions these strain engineering results should be trusted, yielding an enhancement of the figure of merit of nearly two times with respect to the unstrained case
Keywords: Density Functional Theory; 2D materials; nanoscale electronic and thermal transport..

REFERENCES

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FIGURES

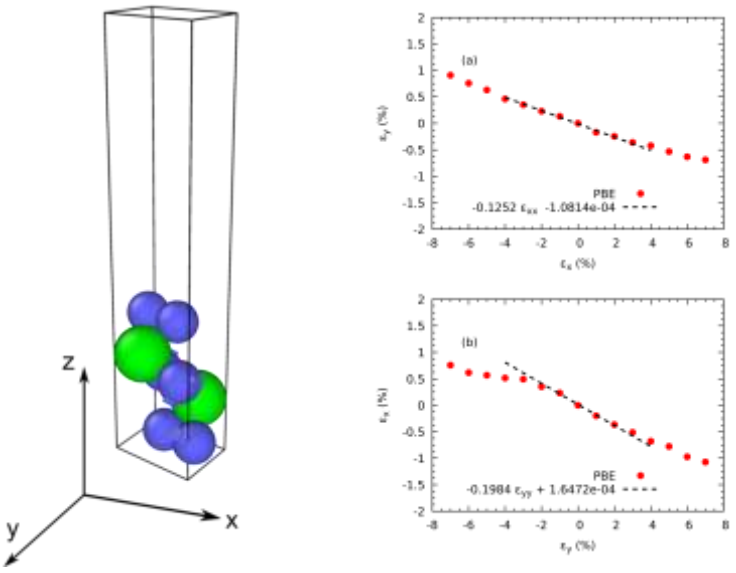

Figure 1: Please make a brief schematic diagram as 'Graphical Abstract'. Insert those Graphics and Synopsis here. Please make sure that this can clearly illustrate your work.