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Supplementary Information: The unexpected effect of vacancies and wrinkling on the electronic properties of MoS_2 layers

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Next we show the structures of the refractory sulphur compounds, a comparison between the predictions of the classical REAXFF and the DFT calculations, the complete Projected Density of States (PDOS) of the 1H phase for compression magnitudes of 0%, 25% and 40%, and a figure similar to figure 5 of the main paper for the 1T′ phase.

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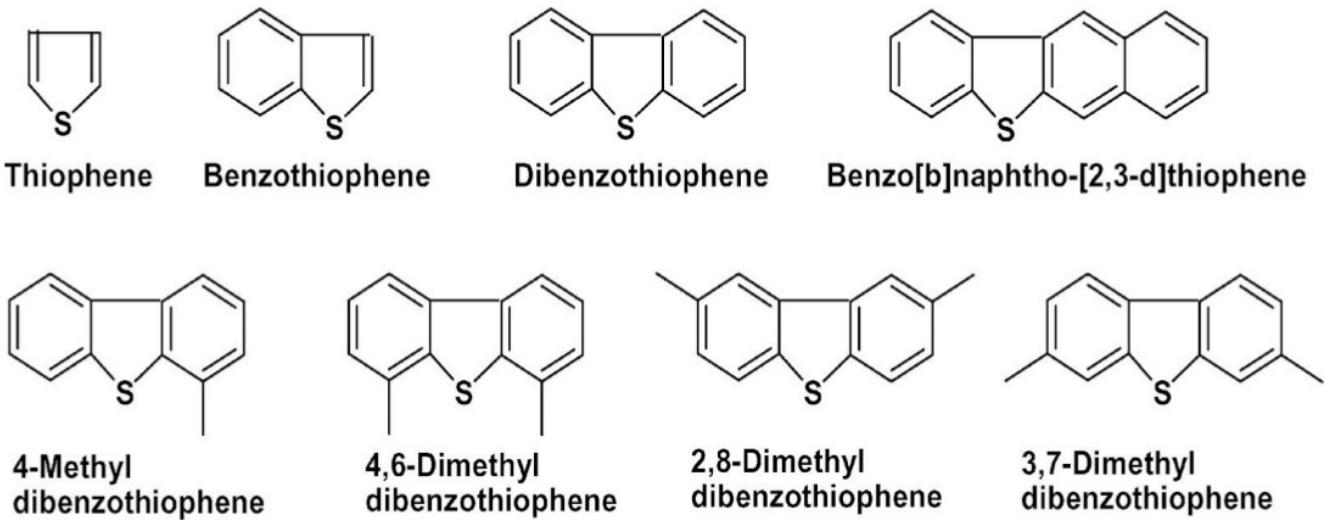

Fig. 1 Structures of the refractory sulphur compounds.

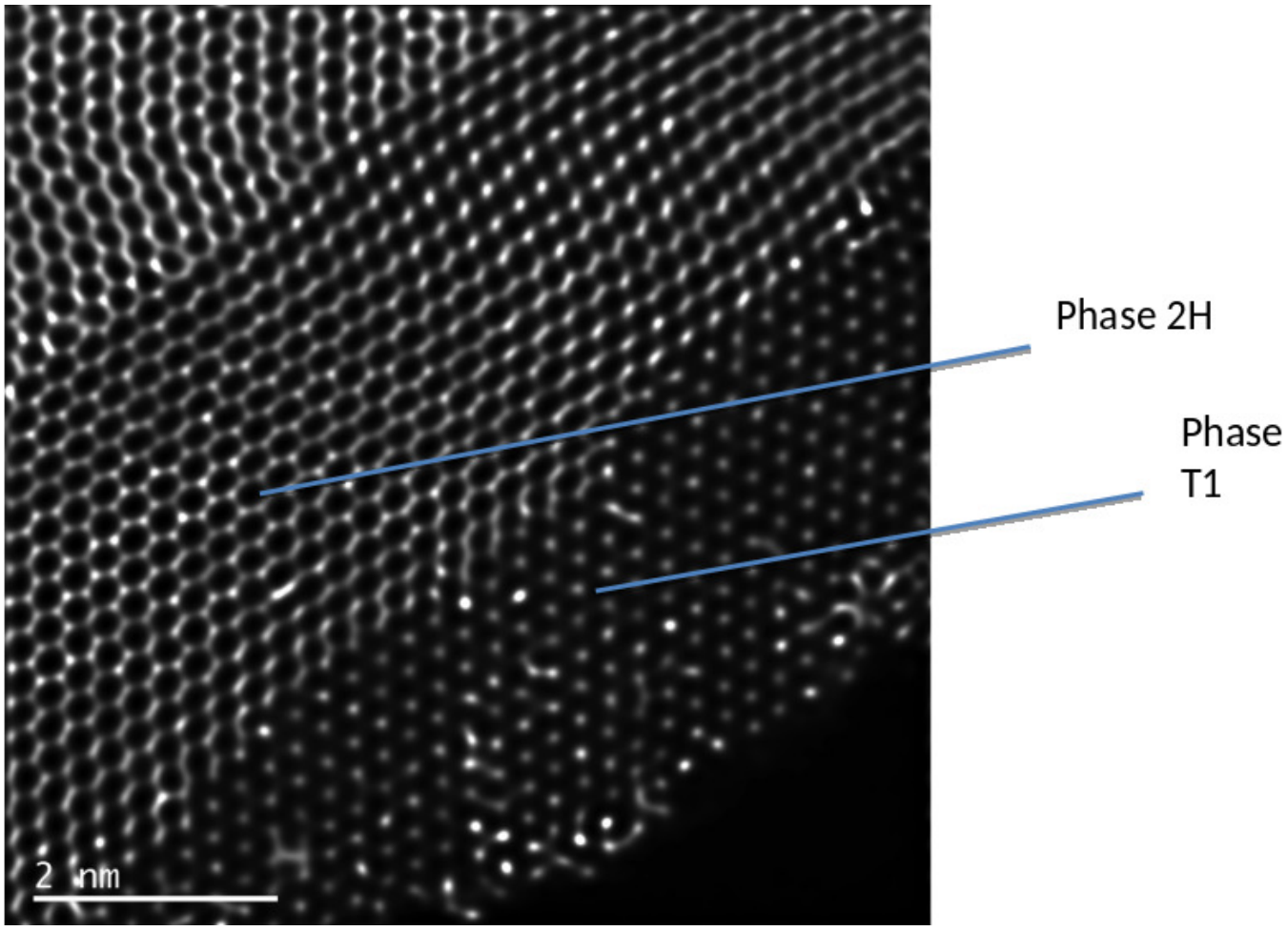

Fig. 2 Image showing the coexistence of the hexagonal and trigonal phases.

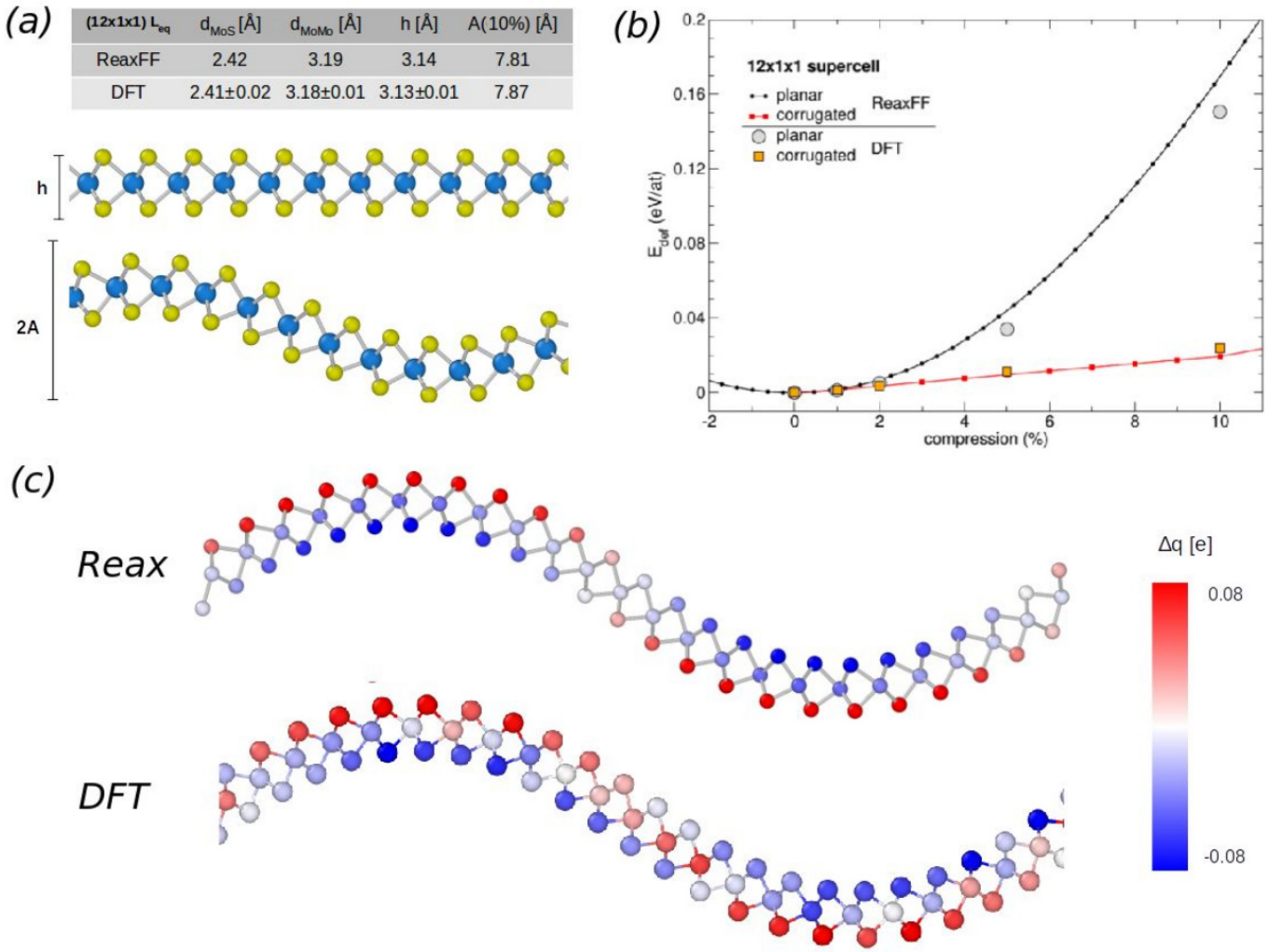

Fig. 3 Comparison between the REAX classical potential and the DFT predictions for the the structural (a), energetics (b) and charge (c) properties of MoS_2 monolayers. In (b), we show the energy per atom in eV for keeping the system planar and allowing it to wrinkle. In (c), blue/red colors mean loss/gain of electrons.

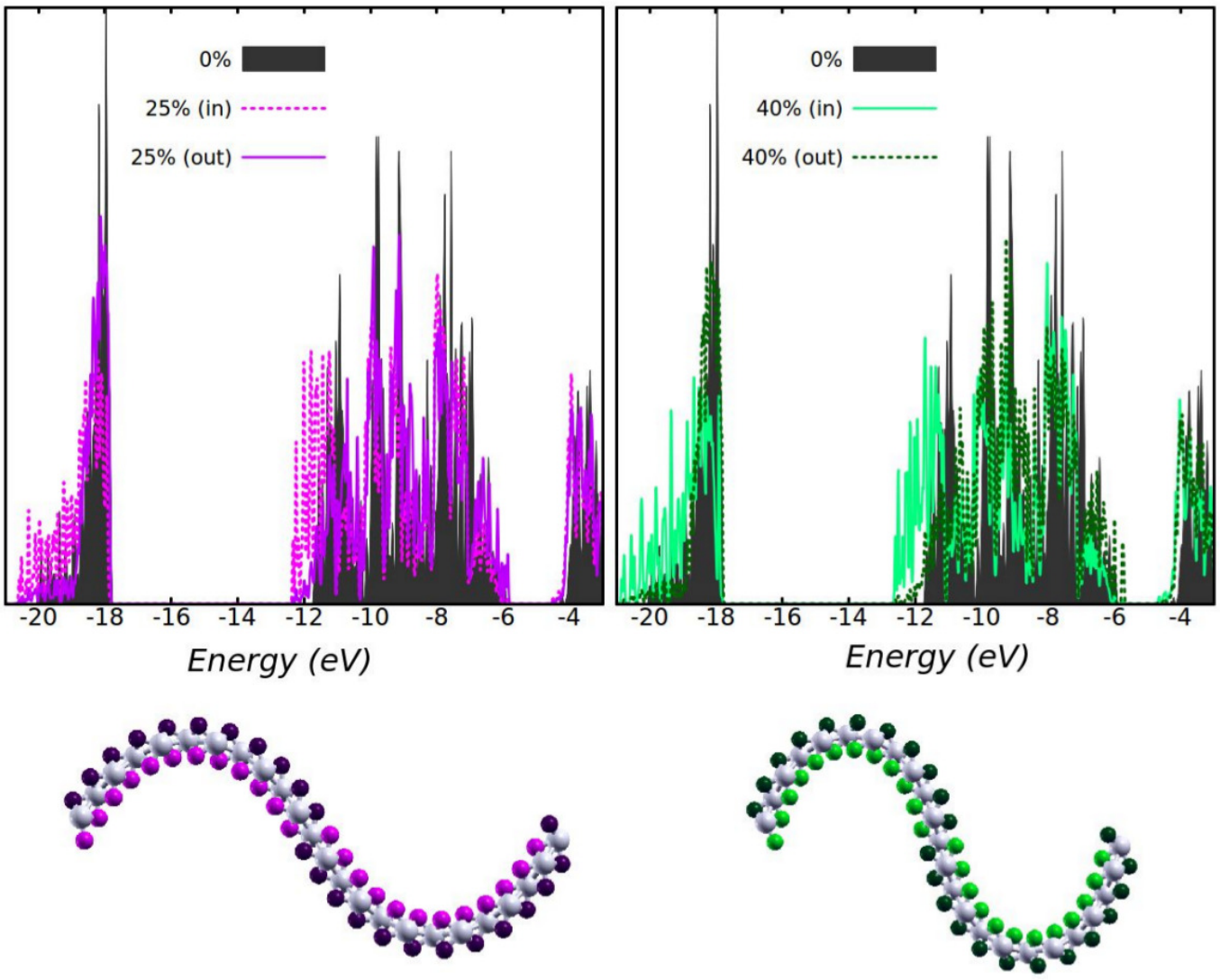

Fig. 4 Complete Projected Density of States (PDOS) for the 1H MoS2 structure with C=0% (dark gray in both figures), with C=25% (left) and 40% (right). The contributions of the internal/ external S atoms is separated with a dashed/continuous line, respectively.

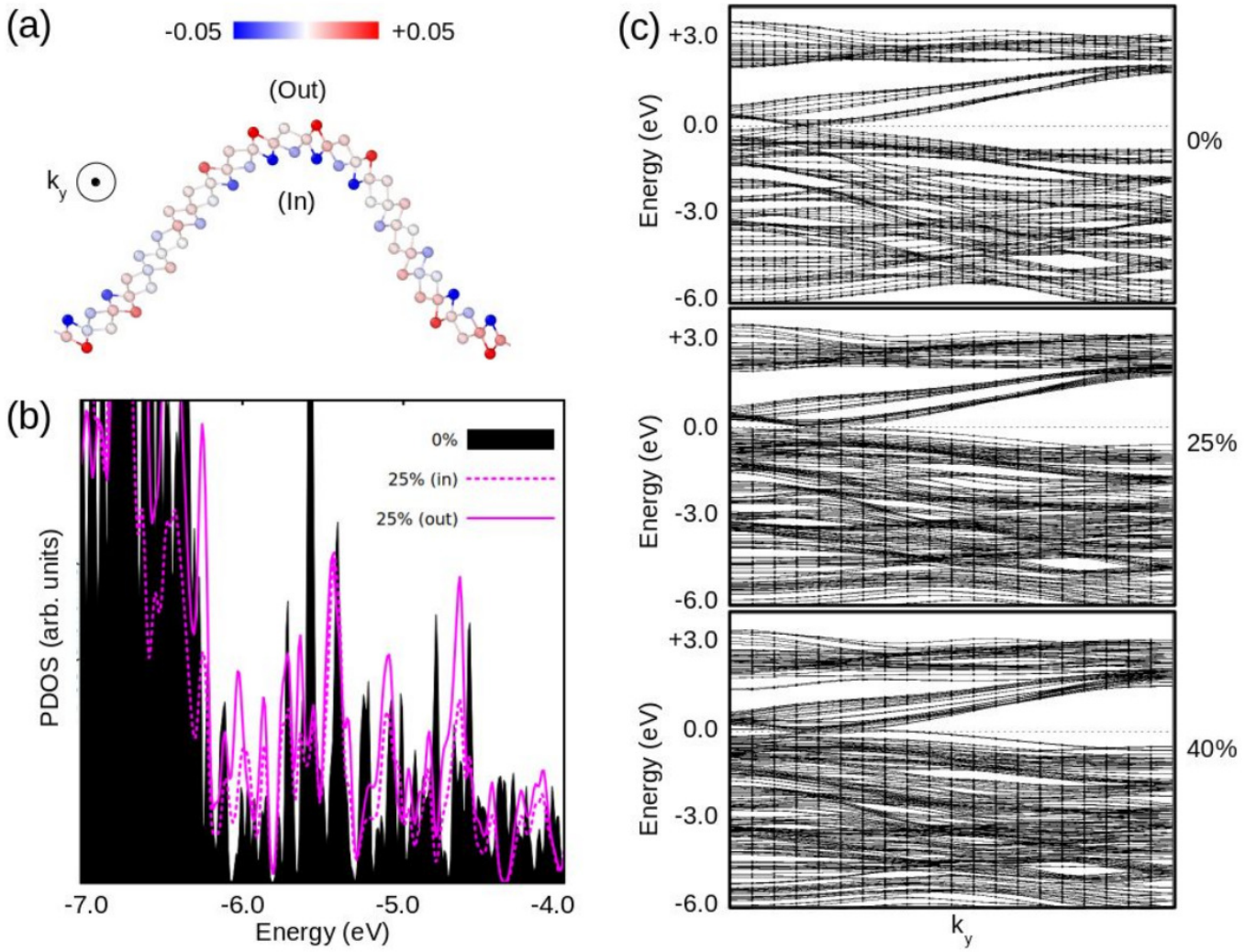

Fig. 5 As it was done in figure 5 of the main paper, we show the electronic properties of wrinkled MoS_2 monolayers in the 1TâĂŹ phase, instead of the 1H. In (a), difference between the atomic charges of the hexagonal planar structure and the 10% compressed structure. Red/blue means gain/loss of charge, and the two groups of S atoms, in the inner and outer curve, are indicated with the In/Out labels. The PDOS for three representative magnitude compressions is shown in (b), separating the contribution of the inner/outer shells. As opposed to what happens for the 1H case, the PDOS shows only a larger contribution of the outer shell, with no shift in energy. The band structure interpolated in the perpendicular ky direction, illustrated in (a), is shown in (c). For each case, we highlight the energy gap value and the reciprocal space direction.