GRAPHENE AND 2DM VIRTUAL CONFERENCE & EXPO

Graphene online 2020 October 19-23

ULTRA-FLAT TWISTED SUPERLATTICES IN 2D HETEROSTRUCTURES

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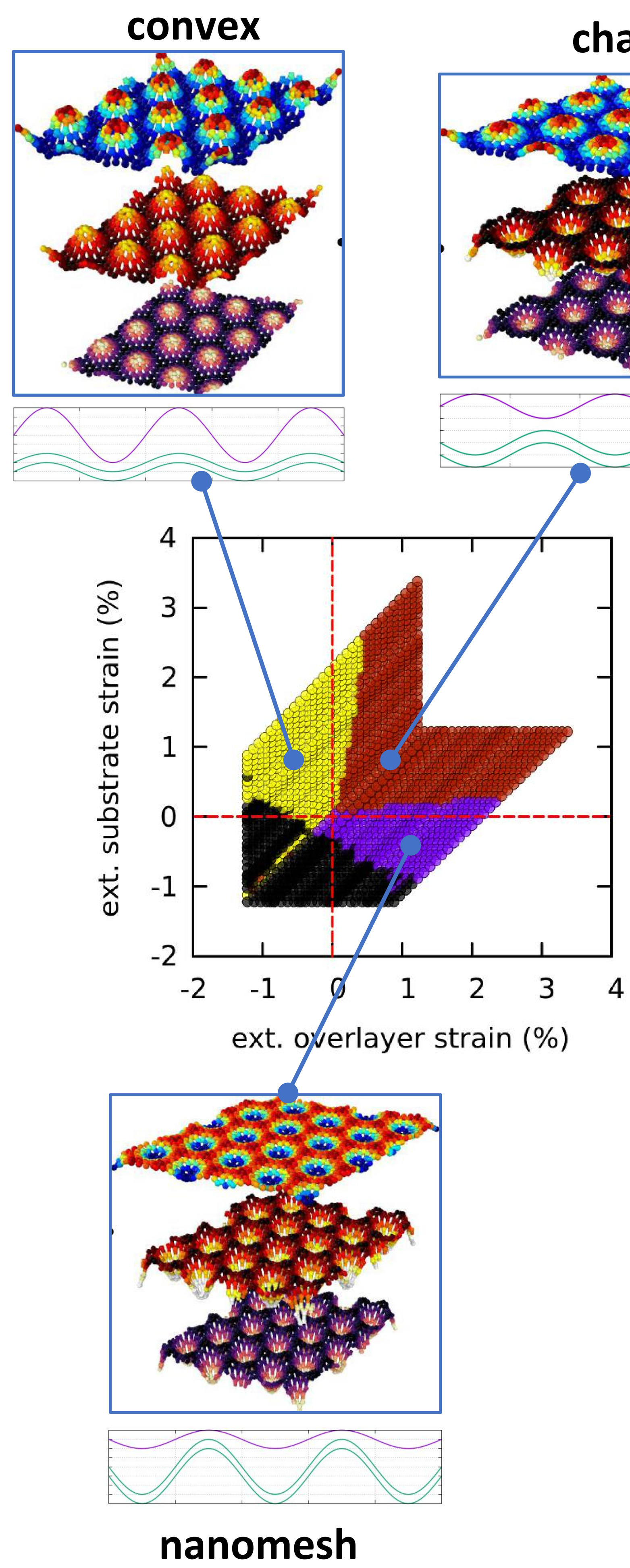
Topographical Moiré-phases

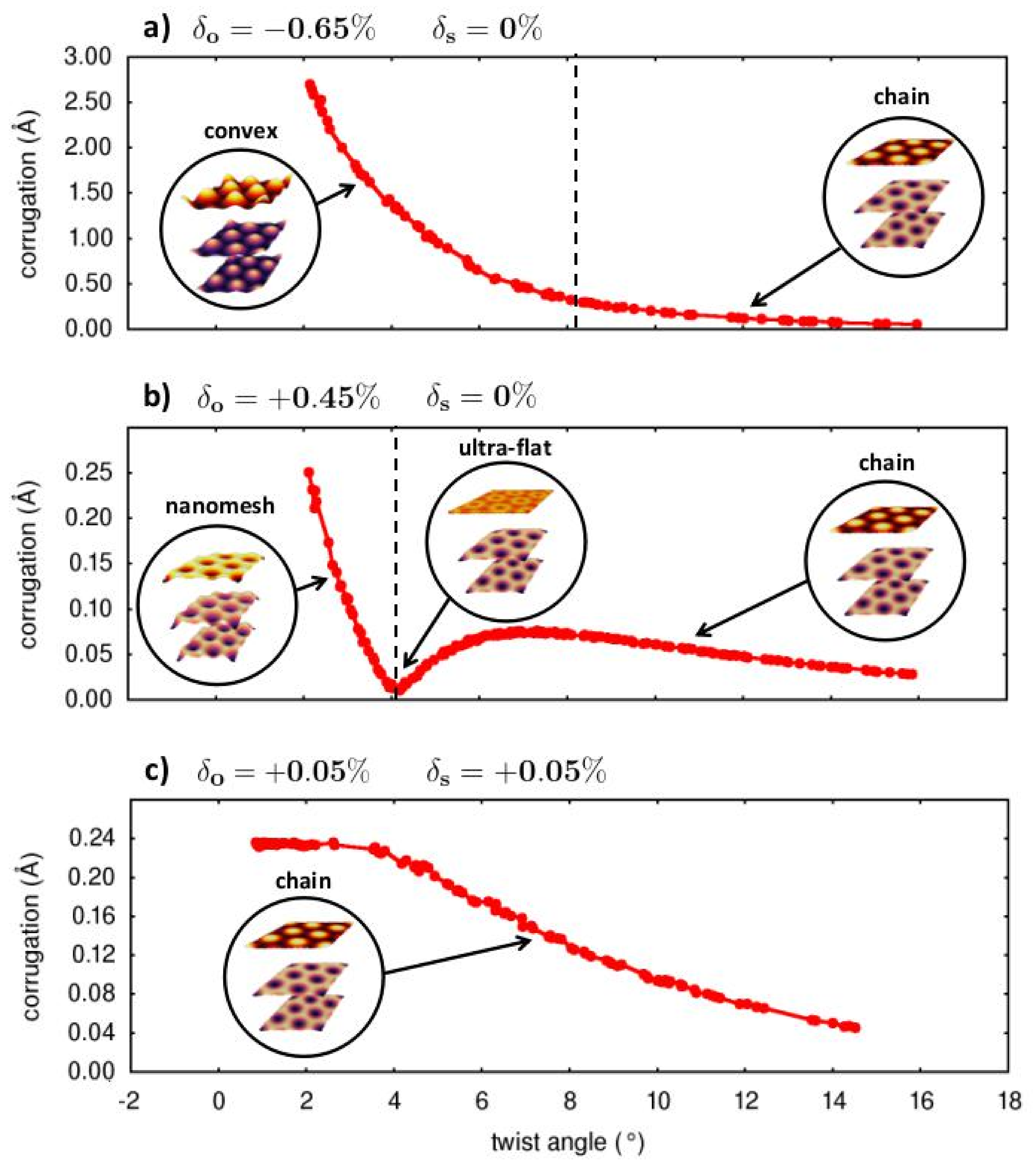
In 2D heterostructures, Moiré superlattice corrugation can develop in both upper and lower layers. The Moiré-amplitude in the substrate can be in phase with the overlayer amplitude (bending modes), or in anti-phase (breathing mode). There are two bending modes (convex, nanomesh) and one breathing (chain), which we call together Moiré-phases. Here we found [1] by lattice relaxation of around 8000 different few-layer graphene Moiré-superstructures using high scale Classical Molecular Simulations, that independently applied external strain to the overlayer and to the substrate is crucially responsible for the realization of the different Moiré-phases.



The Moiré-morphology is defined by the balance between the elastic energy and the vdW adhesion. The elastic energy term is influenced by both the Moiré-wavelength (twist angle) and externally applied strains. The latter can substantially influence the corrugational behavior of the superlattice, leading to different types of Moiré-phase transitions during twist angle alteration. This phenomenon is shown in the figure on the right.

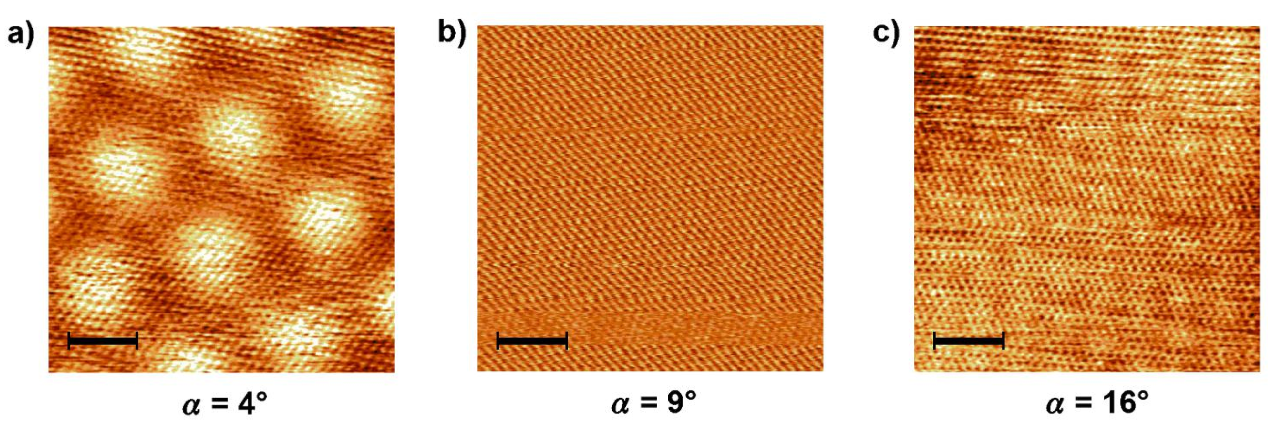
Fig: Moiré-superlattice corrugations of the top rotated graphene layer for three differently strained five-layer graphene heterostructures (red dots) from molecular mechanics simulations. Each point represents a commensurate Moiré-superlattice (δ_o - overlayer strain, δ_s - substrate strain).

Twist induced Moiré-phase transitions



The corrugation can be closely zero (ultra-flat state) (b), constant (c), or even can increase (b) with increasing twist angle depending on the external strain configuration.

STM Investigations



Topographic STM images of graphene layers deposited on top of a graphite substrate for various relative rotation angles (scale bars: 2 nm). Although the apparent corrugation has a decreasing tendency from a–c, the STM image in panel b reveals an ultra-flat state, much smoother than observed even for high rotation angles (c). The experimental conditions for image acquisition (I_{tunnel} = 1 nA, U_{bias} = 200 mV), data processing, and graphic display parameters are the same for all panels.

Ultra-flat states

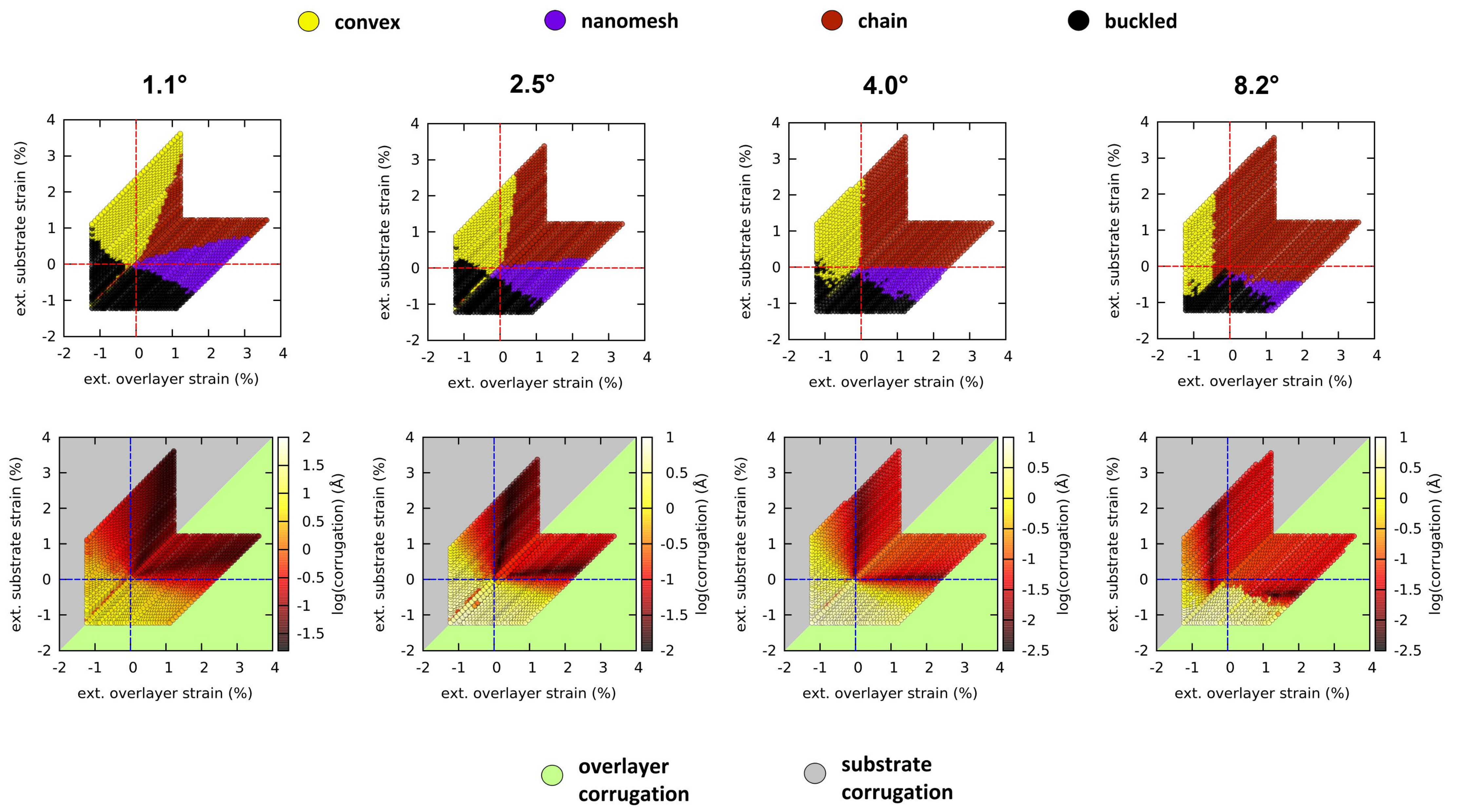


Fig: Moiré-phase maps for different twist angles in the space of externally applied homogeneous strains. a–d A single point in a map represents a relaxed three-layer graphene commensurate Moiré-superlattice. The corresponding Moiré-phases are indicated with different colors (yellow–convex, purple–nanomesh, red–chain). As the twist angle increases the phase boundaries move, and the chain phase becomes dominant. e–h The same phase-maps as a–d, but colored by the corrugation of the relaxed Moiré-superlattices. The dark areas show the ultra- flat states around the phase boundaries. On the side of the green shaded area, the overlayer corrugation is shown, while on the gray side the substrate corrugation is displayed, in order to show the ultra-flat states both in the overlayer and in the substrate.

Acknowledgements

We acknowledge support form NanoFab2D ERC starting grant and NIIF. M.Sz. and P.S. acknowledge funds from NKFIH Grant K-119532. G.D. acknowledges support from the Bolyai fellowship

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https://doi.org/10.1038/s41524-020-00364-w

Graphene online 2020