A first-principles-based multi-scale model for moiré phonons

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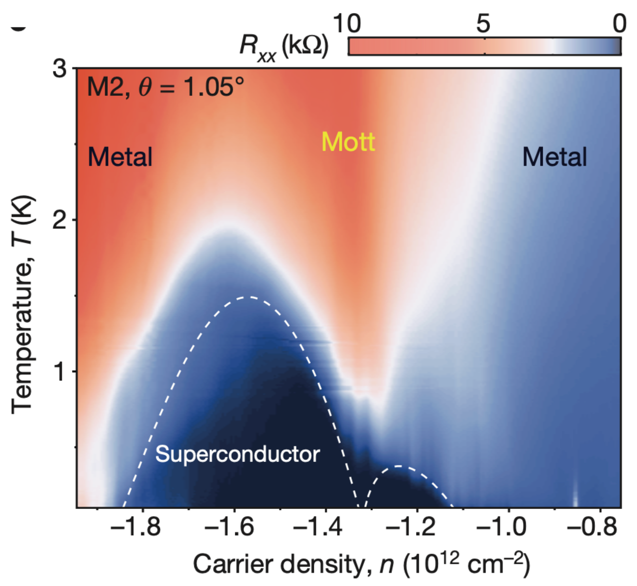
Physical Review B 106 (14), 144305 (2022)

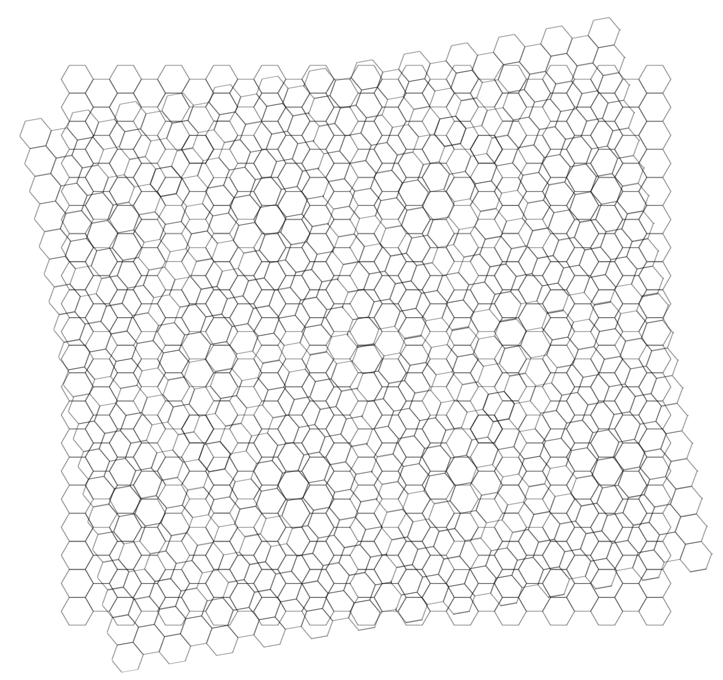
Background

Superconductivity in moiré systems

Twisted bilayer graphene

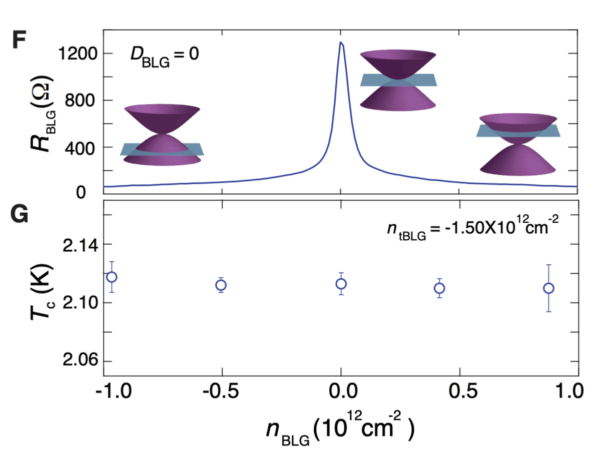


Y. Cao, Pablo Jarillo-Herrero, *et al.*, *Nature* 556, 43–50 (2018)



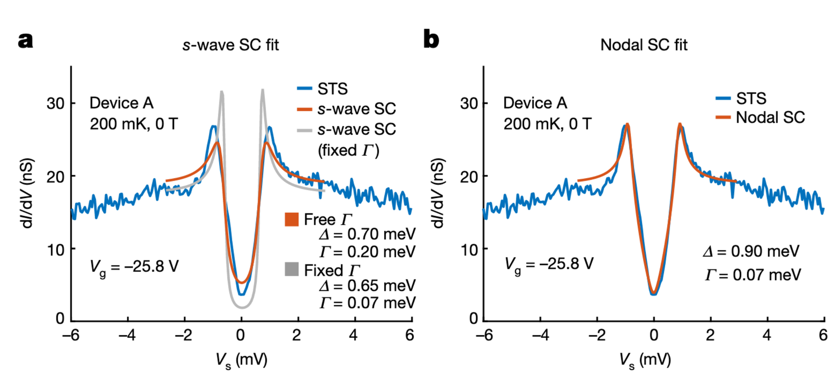
Phonons? **Electrons?**

Tc is insensitive to screening:



X. Liu, Jia Li et al., *Science* 371.6535 (2021): 1261-1265.

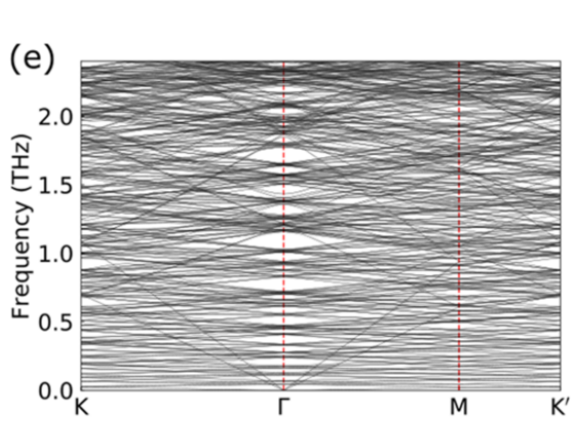
Evidence for nodal superconductivity:



M. Oh, A. Yazdani et al., *Nature* 600.7888 (2021): 240-245.

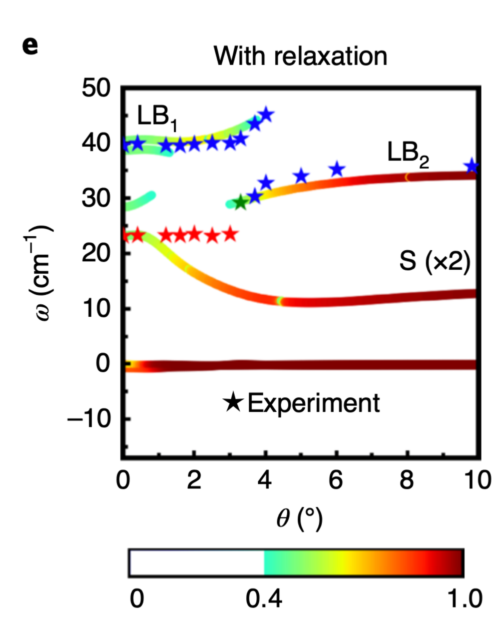
Lack of comprehensive microscopic theory

First-principles calculations (*ab initio* deep potential



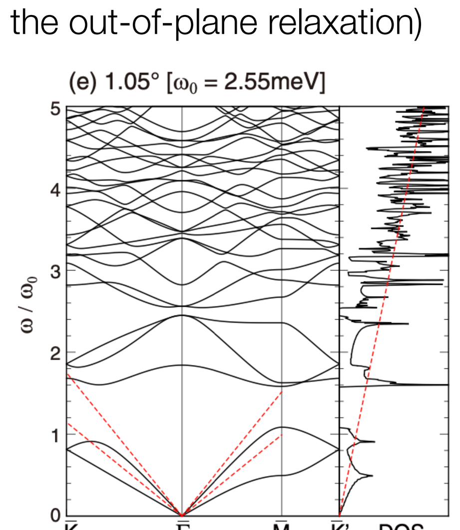
Liu *et al.*, Nano Lett. 2022, 22, 7791-7797

DFT-based continuum model



Quan, Lindhart *et al.*, Nature Materials, 20, 1100–1105 (2021)

Continuum model (neglecting the out-of-plane relaxation)



Koshino and Son, Phys. Rev. B 100, 075416 (2019)

Model challenges

- Large system size
  - Difficult to obtain force fields
- Aperiodicity
  - Cannot use first-principles approach

Configuration space continuum model

Phonon moiré equations of motion

$$\sum_{j\nu\beta\ell'} \overline{D}_{\mu\nu\alpha\beta}(\boldsymbol{R}_i, \boldsymbol{R}_j)\delta\widehat{u}_{j\ell'\nu\beta} = \omega^2 \delta\widehat{u}_{i\ell\mu\alpha}$$

Fourier transform

$$D_{\text{moiré}}(\widetilde{\boldsymbol{k}}) = \begin{bmatrix} D^1(\widetilde{\boldsymbol{k}}) & D^{12} \\ D^{12\dagger} & D^2(\widetilde{\boldsymbol{k}}) \end{bmatrix}$$

μν - atomic indices
αβ - Cartesian coordinates

Phonon scattering selection rule

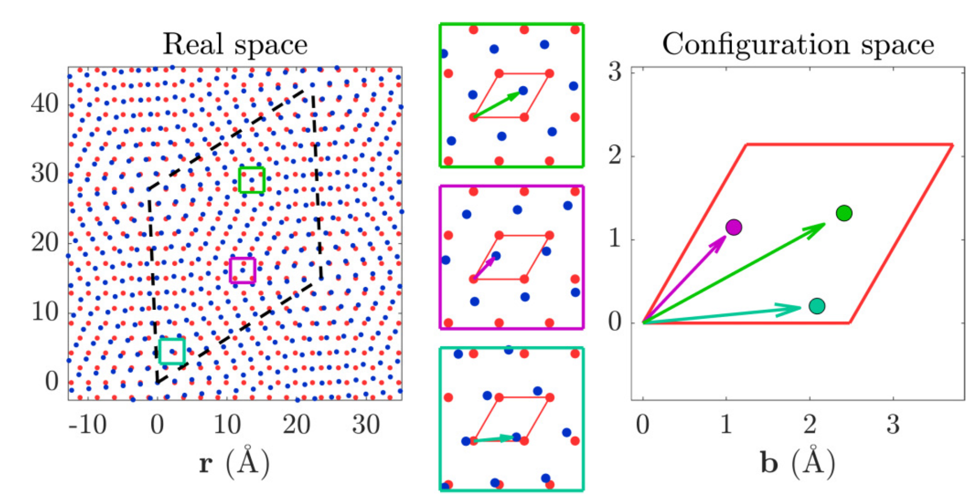
Moiré dynamical matrix element

$$D_{\widetilde{\boldsymbol{k}}\mu\nu\alpha\beta}(\boldsymbol{k}^{(\ell)}, \boldsymbol{k}^{(\ell')}) = \frac{1}{|\Gamma|}\sum_{mn} D_{\mu\nu\alpha\beta}(\widetilde{\boldsymbol{k}} + \boldsymbol{k}^{(\ell)} - \boldsymbol{G}^{(\ell)}_{mn})\, \delta_{\boldsymbol{k}^{(\ell)} - \boldsymbol{k}^{(\ell')}, \widetilde{G}_{mn}}$$

Moiré reciprocal lattice

In analogy to the electronic structure selection rule (Bistritzer and MacDonald model)

Obtaining the matrix element: configuration space



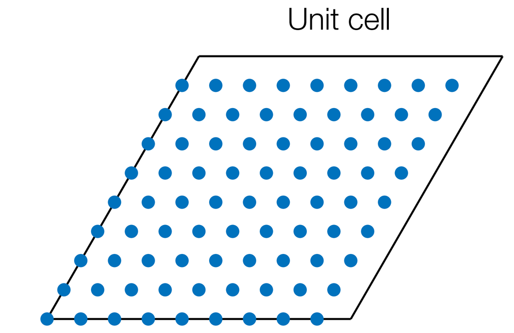
$$\boldsymbol{b}(\boldsymbol{r}) = \left(\mathbb{1} - A_2 A_1^{-1}\right)\boldsymbol{r}$$

Carr *et al.*, PRB 98 224102 (2018)

$$D^{\text{rig}}_{\mu\nu\alpha\beta}(\widetilde{\boldsymbol{k}} + \widetilde{\boldsymbol{G}}) = \frac{1}{N^2}\sum_{\boldsymbol{b}\in S(N)} D^{(\boldsymbol{b})}_{\mu\nu\alpha\beta}(\widetilde{\boldsymbol{k}})e^{i(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{b}}$$

Dynamical matrix at configuration b

Unit cell

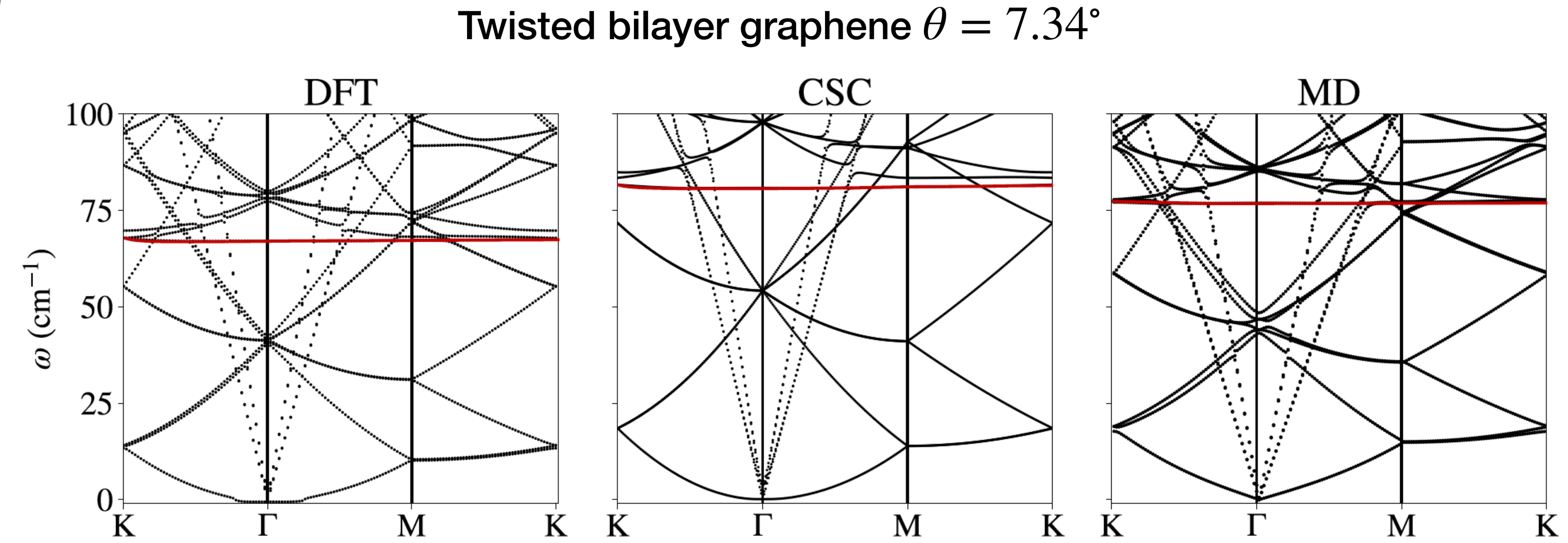


$S(N)$ - the uniform grid

Relaxation - non-uniform grid

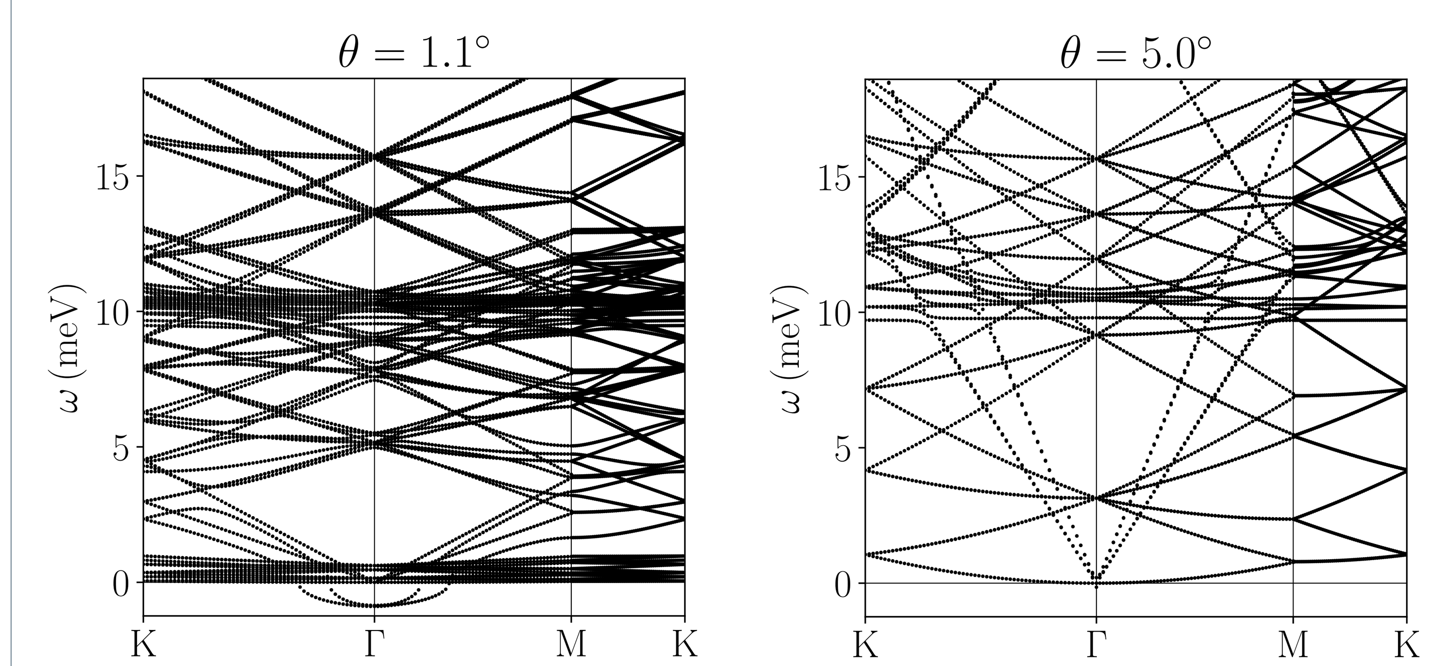
Model validation

Twisted bilayer graphene $\theta = 7.34°$

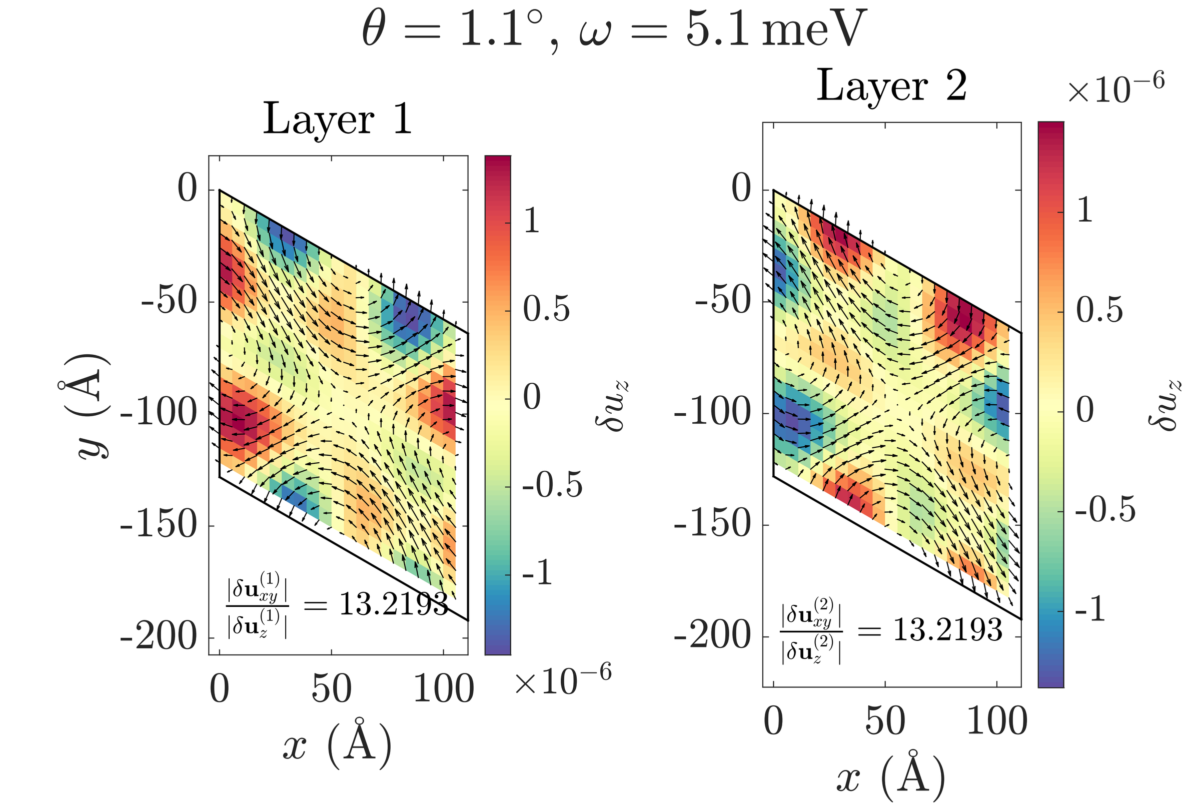


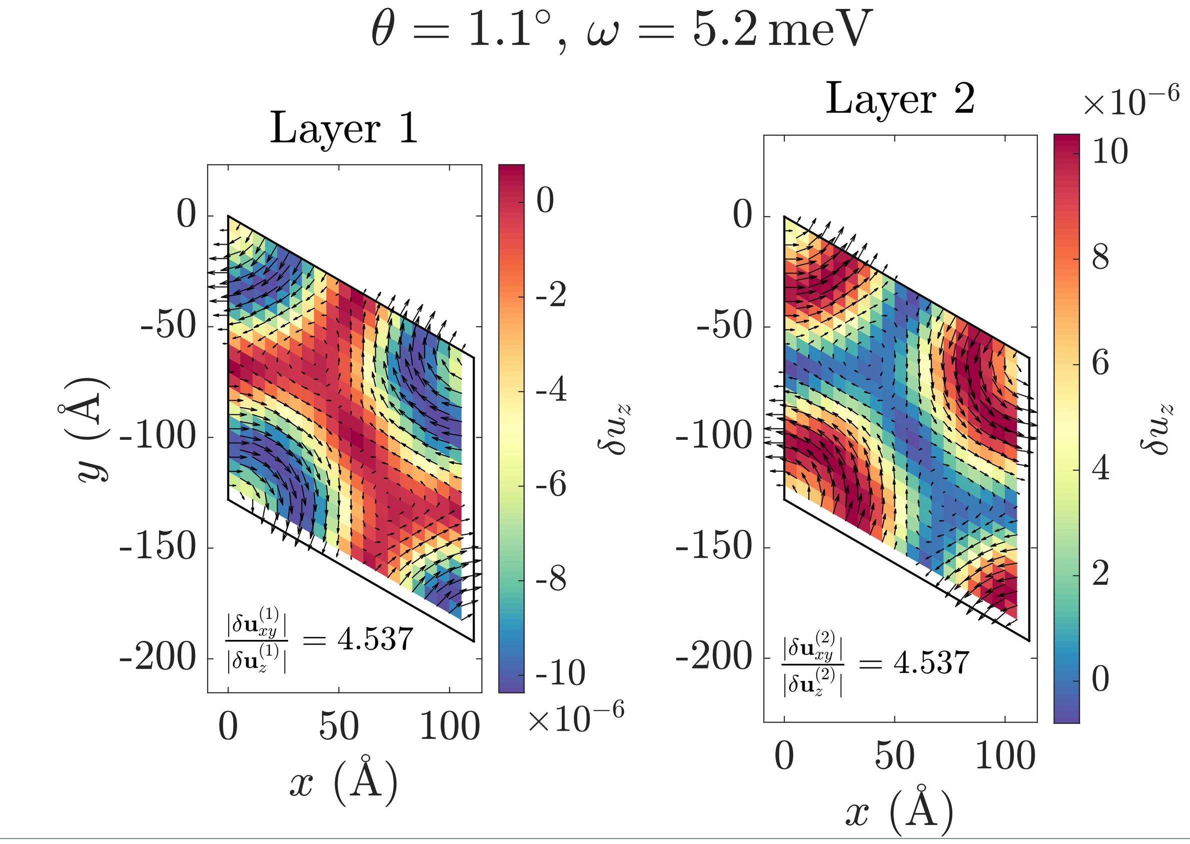
Phonon mods

Twisted bilayer graphene band structure



Γ point phonon





Summary

- Developed a first-principles-based continuum model for moiré phonons based on configuration space, bypassing expensive force fields calculations and generic to all twist angles and materials
- Benchmarked against first principles calculations, showing good agreement

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