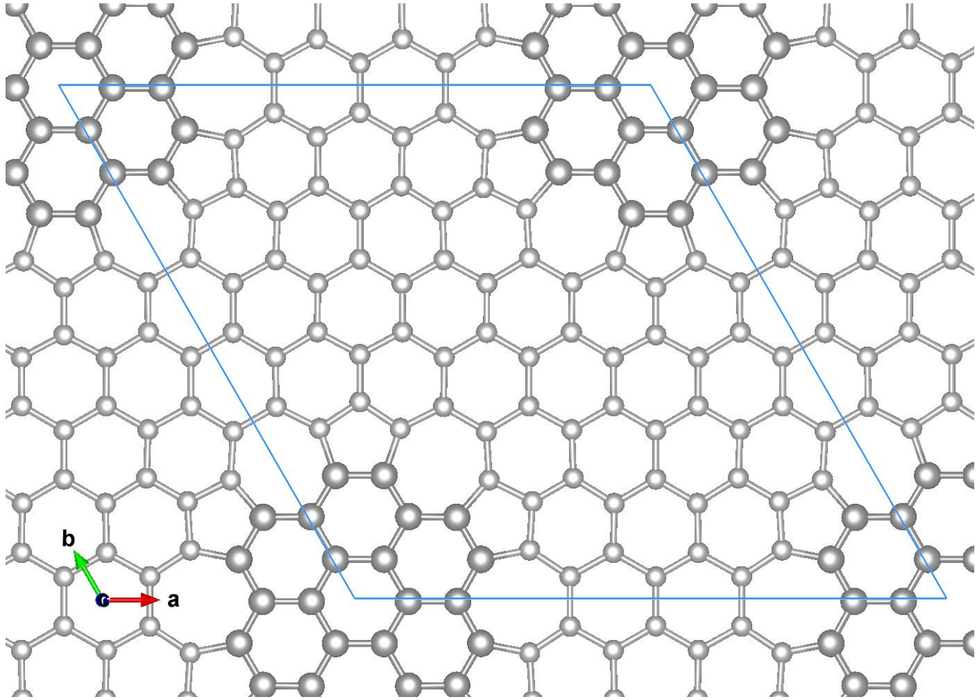

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First principles studies of 7x7 graphene superlattices with topological defects and transition metal adatoms

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Introduction

- Graphene's lack of a bandgap and magnetism limits its applications.
- However, Topological defects, such as flower-like defects (FLDs) observed via STM [1], can modify its electronic and magnetic properties. Certain 1D extended defects also show unique behaviors like 1D conductivity [2].
- A systematic study of graphene's structural, mechanical, electronic, and magnetic properties is thus crucial to overcome these limitations. Here, we propose and investigate a hexagonal array of FLDs forming a 7×7 superlattice.

Methodology

- Calculations were performed using VASP [3], employing the R2SCAN+rvv10 functional [4]. Visualizations were generated using VESTA [5].
- We used a 900 eV plane-wave cutoff and a k-point mesh spacing of 0.022 $Å^{-1}$ for both pristine graphene and the 7×7 FLD superlattice.

VASP

VESTA
Visualization for Electronic and STructural Analysis

Pristine

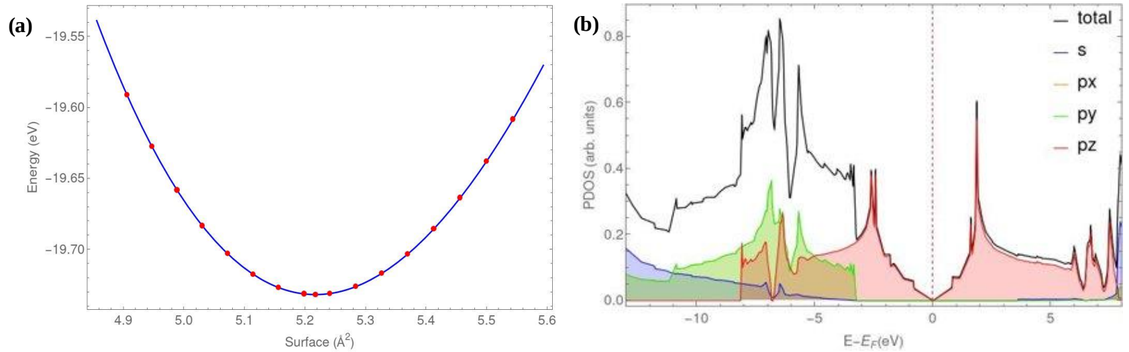

Fig. 1. (a) Energy equation of state (EOS) for pristine. (b) Partial density of states for pristine.

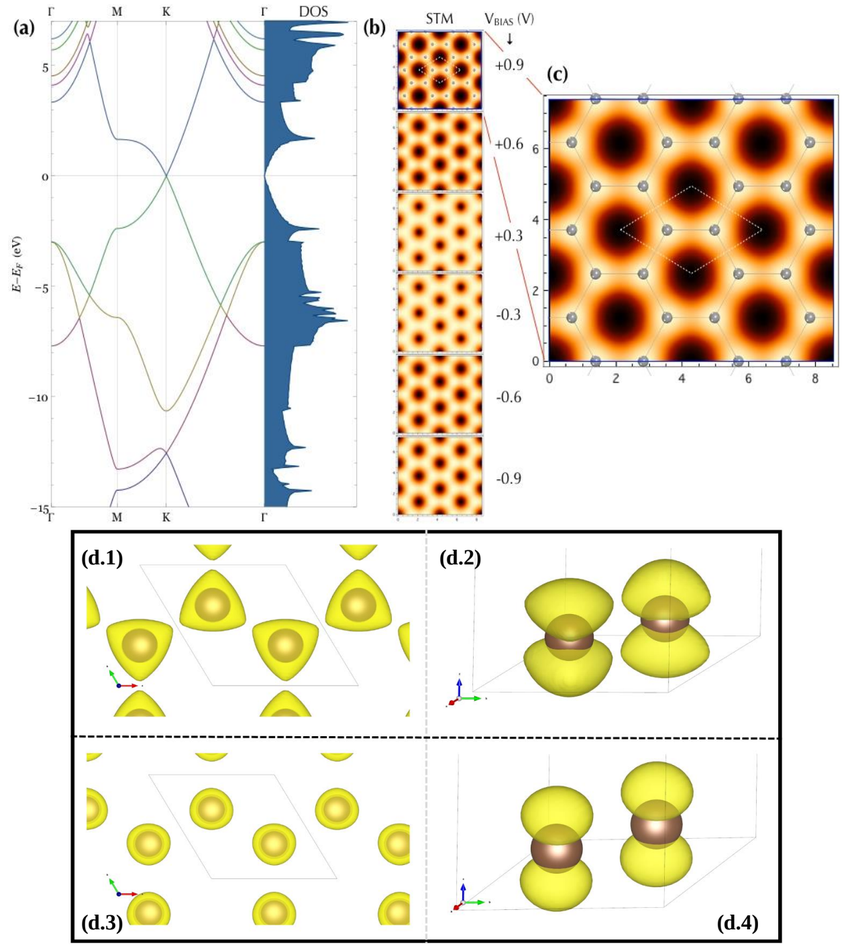

Fig. 2. (a) Band Structure and Density of States (DOS) for pristine. (b, c) Simulated STM images for each corresponding V_{BIAS}.
(d.1, d.2) Isosurface images of partial charge density of last occupied band.
(d.3, d.4) Isosurface images of partial charge density of first unoccupied band.

Results

(a)

System	a_{opt}	N_{atom}	$\gamma\,(eV/Å^2)$	γ'	$\gamma''(Å^2/eV)$	E_{gap}
Pristine	2.45	2	13.51	4.47	-0.34	0
7x7	17.26	98	13.24	4.36	-0.35	0

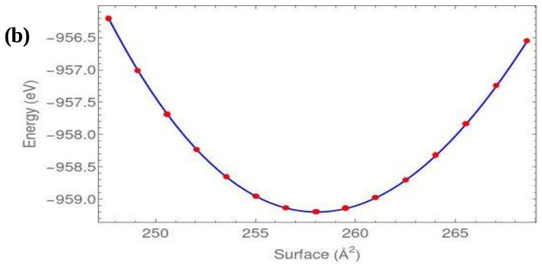

Fig. 3. (a) Results of calculations for pristine graphene and 7x7 arrangement using the EOS [4]. (b) Energy equation of state (EOS) for 7x7 arrangement.

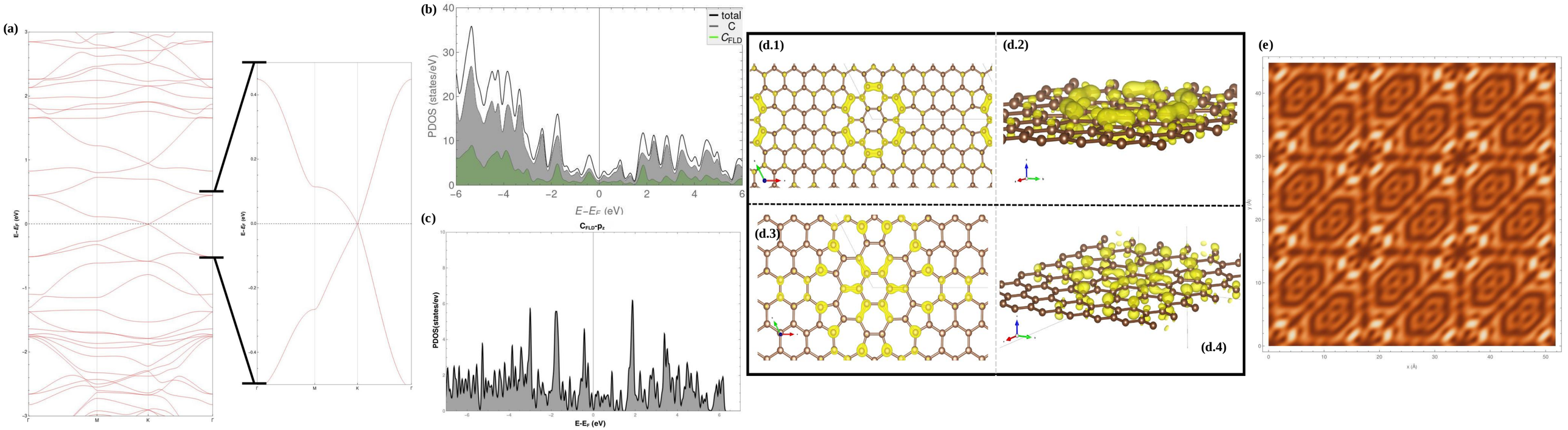

Fig. 4. (a) Band Structure of 7x7 superlattice. (b) Partial density of states (PDOS)of 7x7 superlattice. (c) PDOS of FLD constituent C atoms. (d.1, d.2) Isosurface images of partial charge density of last occupied band. (d.3, d.4) Isosurface images of partial charge density of first unoccupied band. (e) Computed STM for hexagonal array of defects with pattern 7x7 for V_{BIAS}=*-0.3 eV.*

Conclusion and future insights

Future work will explore vacancies in the arrangement, incorporate transition metal adatoms at the different non-equivalent sites, and investigate the effects of adding a new layer in different non-equivalent configurations.

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