LANCASTER UNIVERSITY

Binding energy of bilayer graphene

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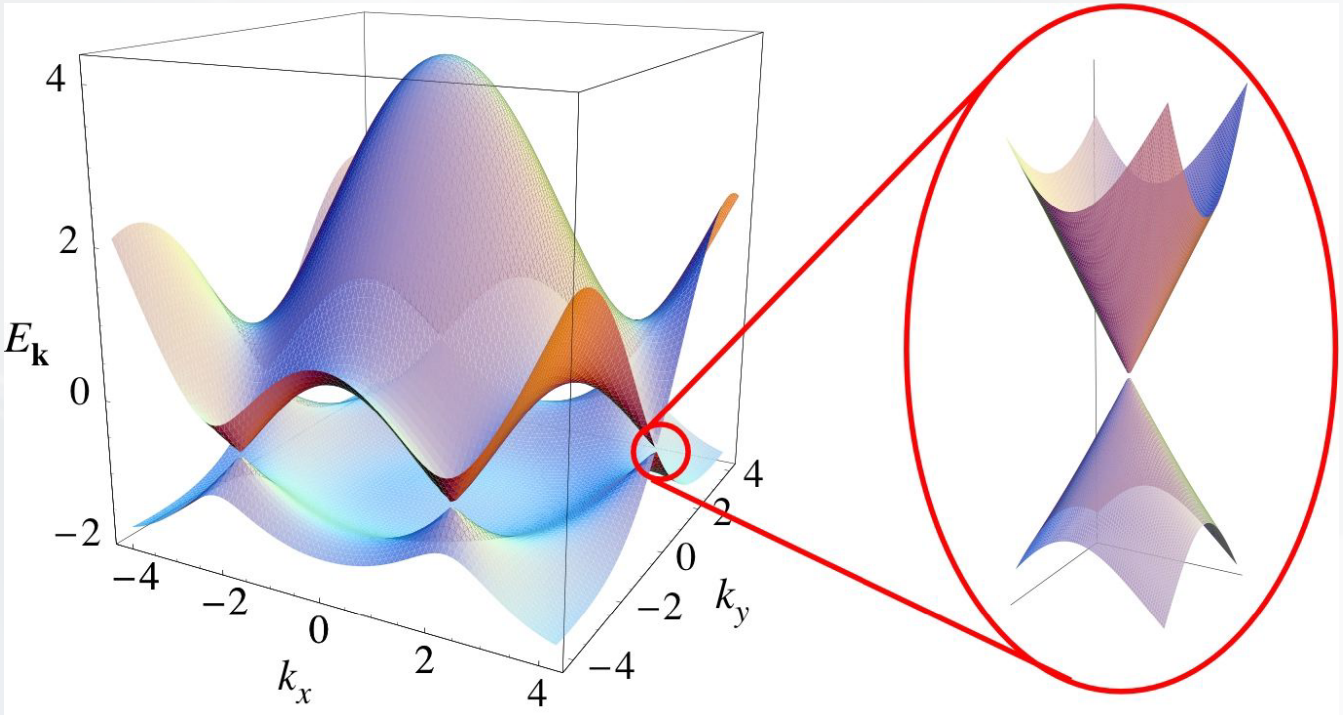
Outline

- Graphene properties and applications
- Method
- Results
- Summary

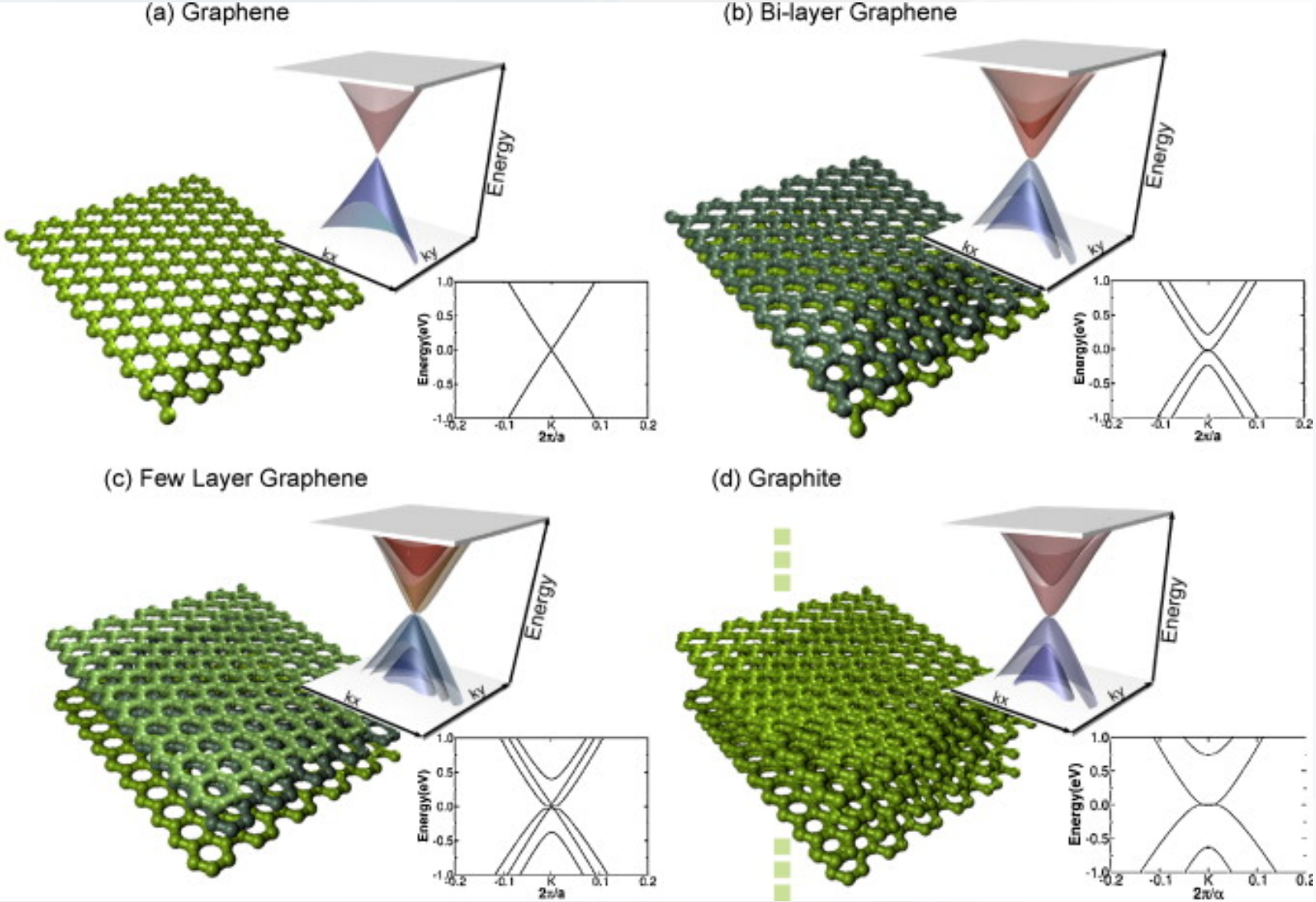
Graphene

- zero band-gap semiconductor
- linear dispersion for electrons (holes) in the conduction (valence) bands.
- Fermi velocity roughly 10^8 cm/s



A. H. Castro Neto *et al.*, Rev. Mod. Phys., **81** (2009).

Graphene layers



M. Terrones *et al.*, Nano Today **5**, 351—372 (2010)

Applications

WELCOME TO THE GRAPHENE AGE

George Osborne on a visit to the Manchester University lab of Professors Geim and Novoselov

SOLAR PANELS

MIT professors have shown how graphene could be used to make the electrodes in organic solar cells cheaper, lighter and more flexible than in current systems

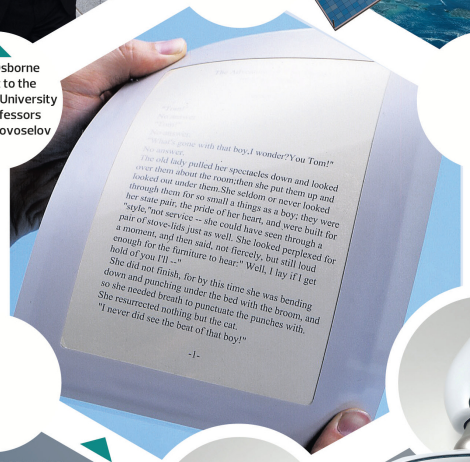
AIR TRAVEL

Using graphene would enable aeroplane manufacturers to develop extremely strong yet light components – bringing down weight and therefore reducing fuel costs

MOBILE PHONES

Nokia is exploring the potential uses of graphene in mobile devices. Aside from smaller, more flexible phones, it may allow built-in solar power and transparent electronics

A CLOSER LOOK AT GRAPHENE



FLEXIBLE SCREENS

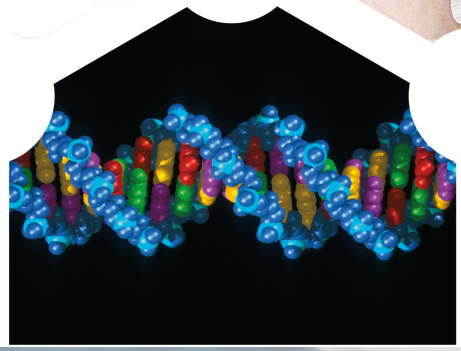
Researchers in South Korea have produced a continuous layer of graphene 63cm wide. This has opened up possibilities in electronics. "You could theoretically roll up your iPhone and stick it behind your ear like a pencil," claims one scientist

PROSTHETICS

Aside from allowing for the construction of stronger, more flexible and lighter limbs, its conductivity opens up new possibilities for its use in the electrodes used to turn brain signals into movement

COMPUTER CHIPS

Geim and Novoselov have been working on demonstrating how graphene could replace silicon as the key material in electronic circuits. IBM is one of many electronics firms experimenting with graphene conductors



DNA SEQUENCING

Researchers at British firm Oxford Nanopore, building on discoveries made at Harvard, claim that using graphene could reduce the cost and speed up the process of DNA sequencing

GRAPHIC: PETE GUEST

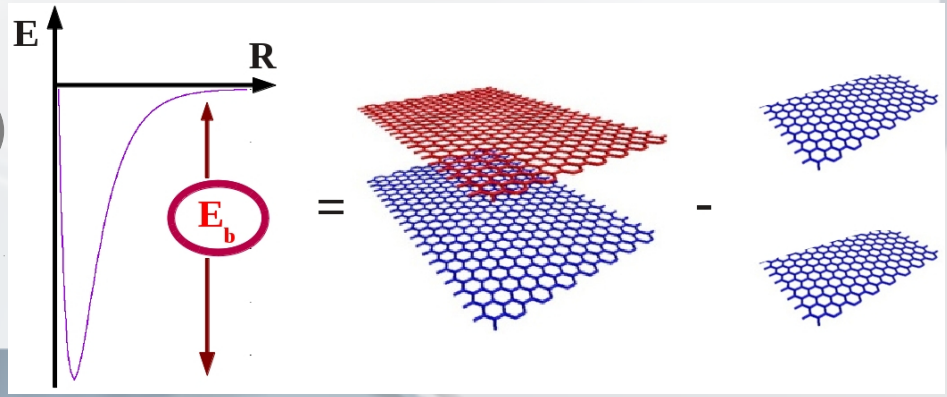
Recent attractive issues

Modelling graphene devices interacting with other 2D materials

Fabrication of superconductors by graphene

Fabrication of upercapacitors by graphene

Binding energy ????



Binding energy(mev/atom)

different Methods

Method	d(Å)	Basis	Functional	k-point	E_b
Graphite					
ACFD_RPA[a]	3.34	PW		14 14 14	62
ACFDT_RPA[b]	3.34	PW	GGA_PBE	10 10 5	48
vdW_DF[c]	3.6	PW	rev_PBE	2 2 2	45.5
QMC [d]	3.426	Gaussian		2 2 2	56
Collapsed carbon nanotube[e]	3.35				35
Self-retraction[f]	3.6				31
Graphene					
vdW-DF (AB)[g]	3.4	PW	PBE	24 36 1	29.3
DFT-D (AB) [g]	"	"	PBE-D	"	50.6
vdW-DFT(AA)[g]	"	PW	PBE	"	18.9
DFT-D (AA) [g]	"	"	PBE-D	"	19.5

[a]. T. Olsen and K. S. Thygesen, Phys. Rev. B **87**, 075111 (2013).
[b]. S. Lebegue *et al.*, Phys. Rev. Lett. **105**, 196401 (2010).
[c]. S. D. Chakarova-Kack *et al.*, Phys. Rev. Lett. **96**, 146107 (2006).
[d]. L. Spanu *et al.*, Phys. Rev. Lett. **103**, 196401 (2009).
[e]. L.X. Benedict *et al.*, Chem. Phys. Lett. **286**, 490 (1998).
[f]. Z. Liu *et al.*, Phys. Rev. B **85**, 205418 (2012).
[g]. I.V. Lebedeva *et al.*, Phys. Chem. Chem. Phys. **13**, 5687 (2011).

Method

- Dirac-Fock pseudopotentials
- DFT calculations for initial single particle wave functions
- VMC and DMC including Jastrow factors
- 3 ×3, 4×4, 5×5, 6×6 and 9 ×9 unit cells

Method

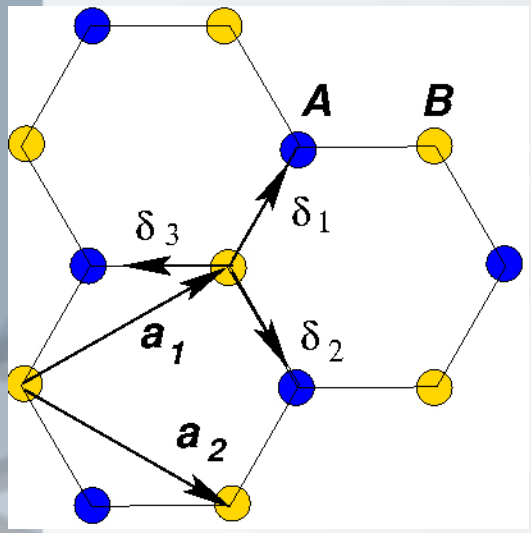
- Twist average to consider more k vectors
- DMC extrapolation to zero time-step
- Exterapolation to infinite system size[1]

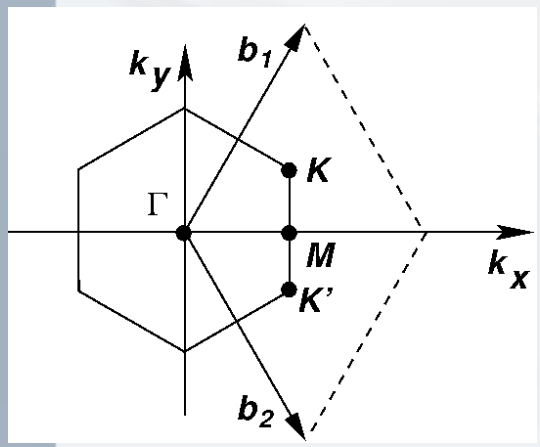
$$E(N) = E(\infty) + bN^{(-5/4)}$$

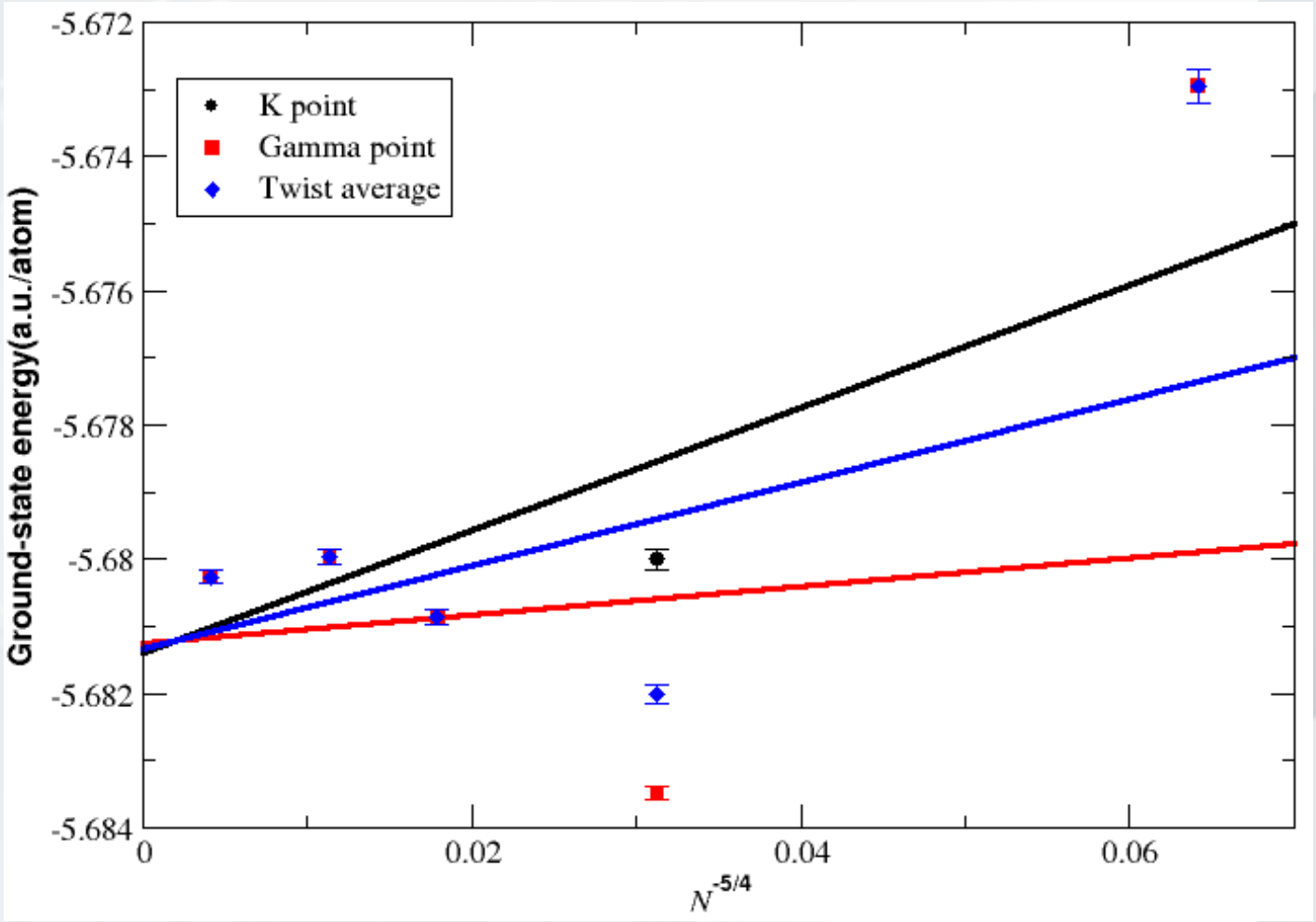
Fitting parameter defined by fitting to QMC

1. Neil D. Drummond *et al.*, Phys. Rev. B **78**, 125106 (2008)

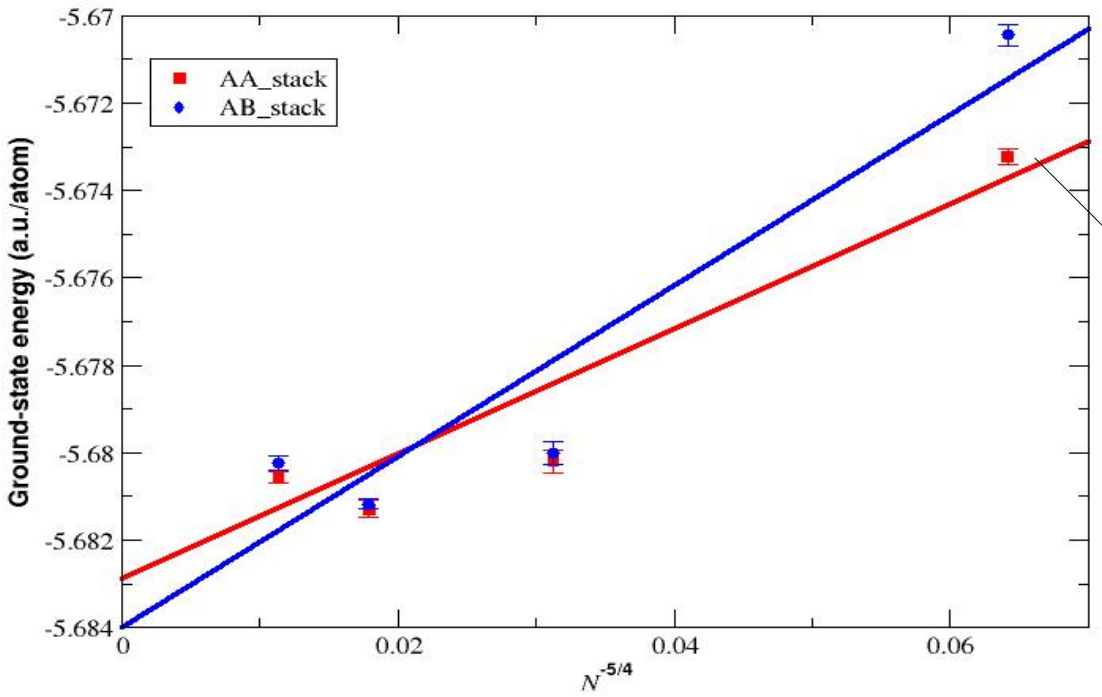
Ground-state energy
for monolayer

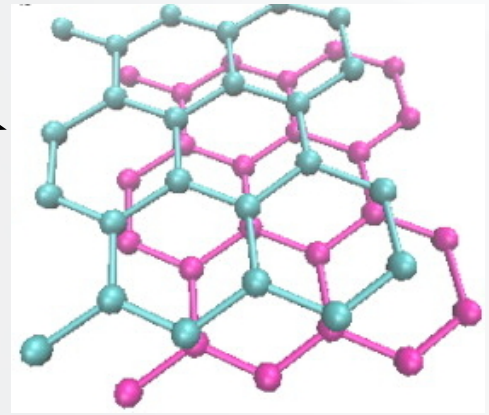


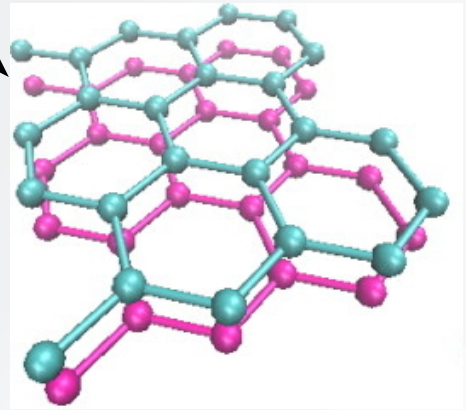




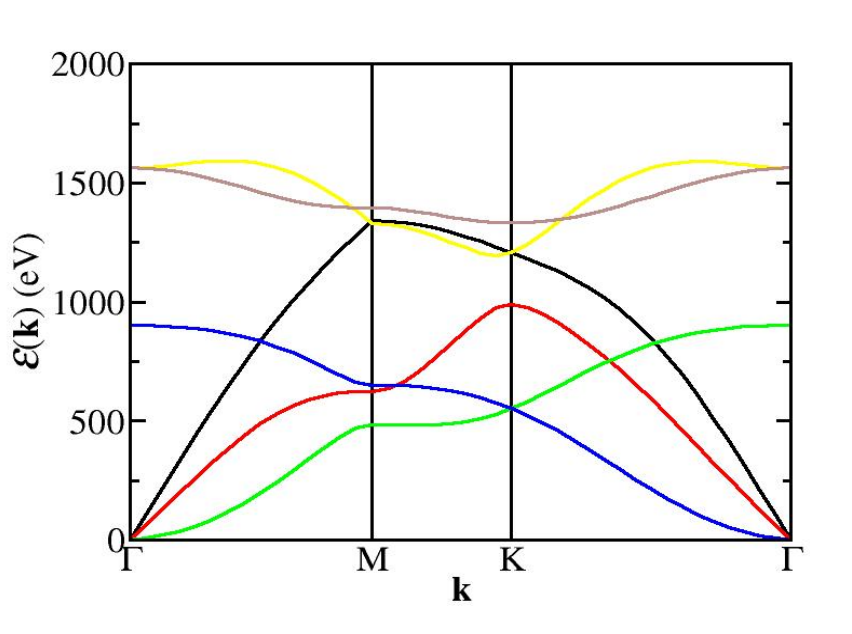
Ground-state energy
for bilayer no twist average

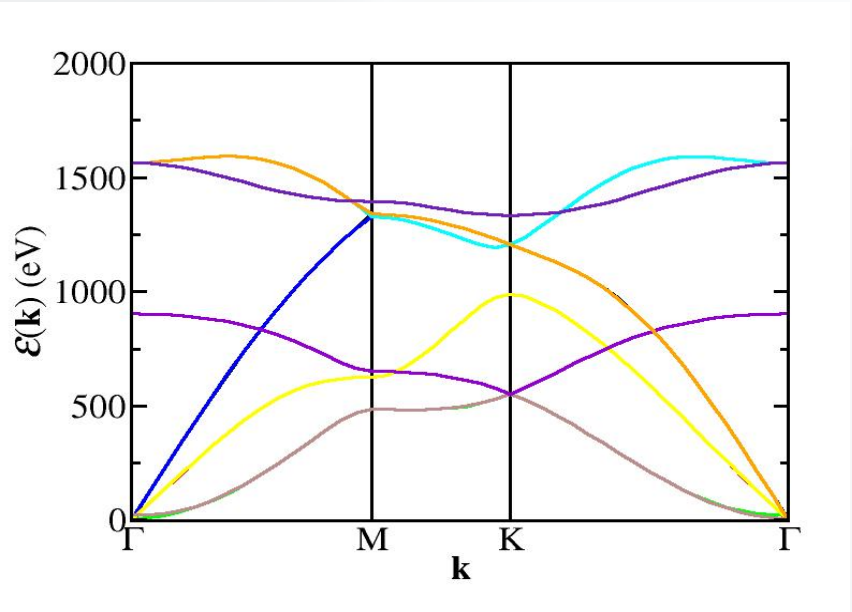






Core vibration effect
negligible



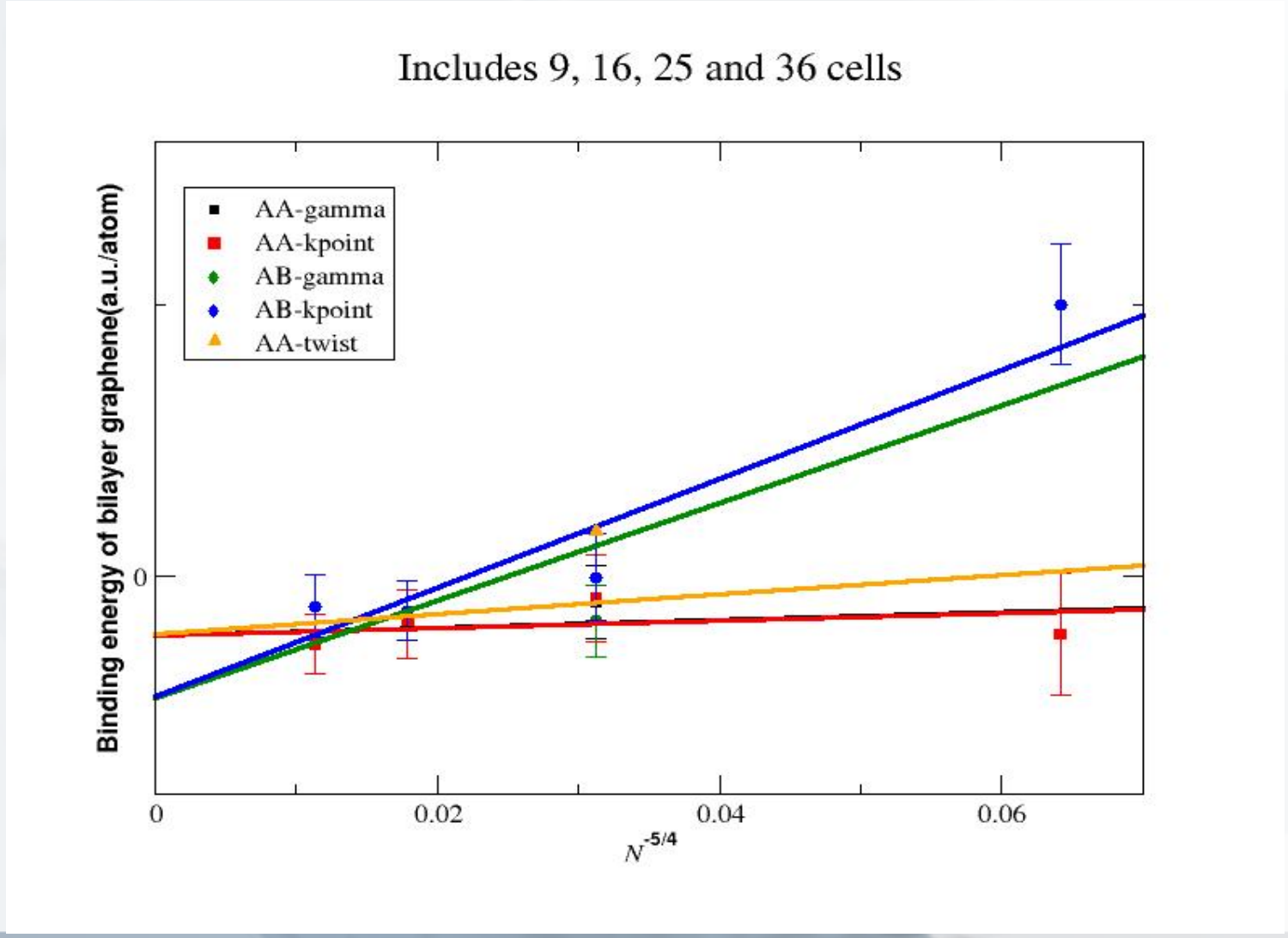


Monolayer zero energy:
0.0126 a.u./prim.cell

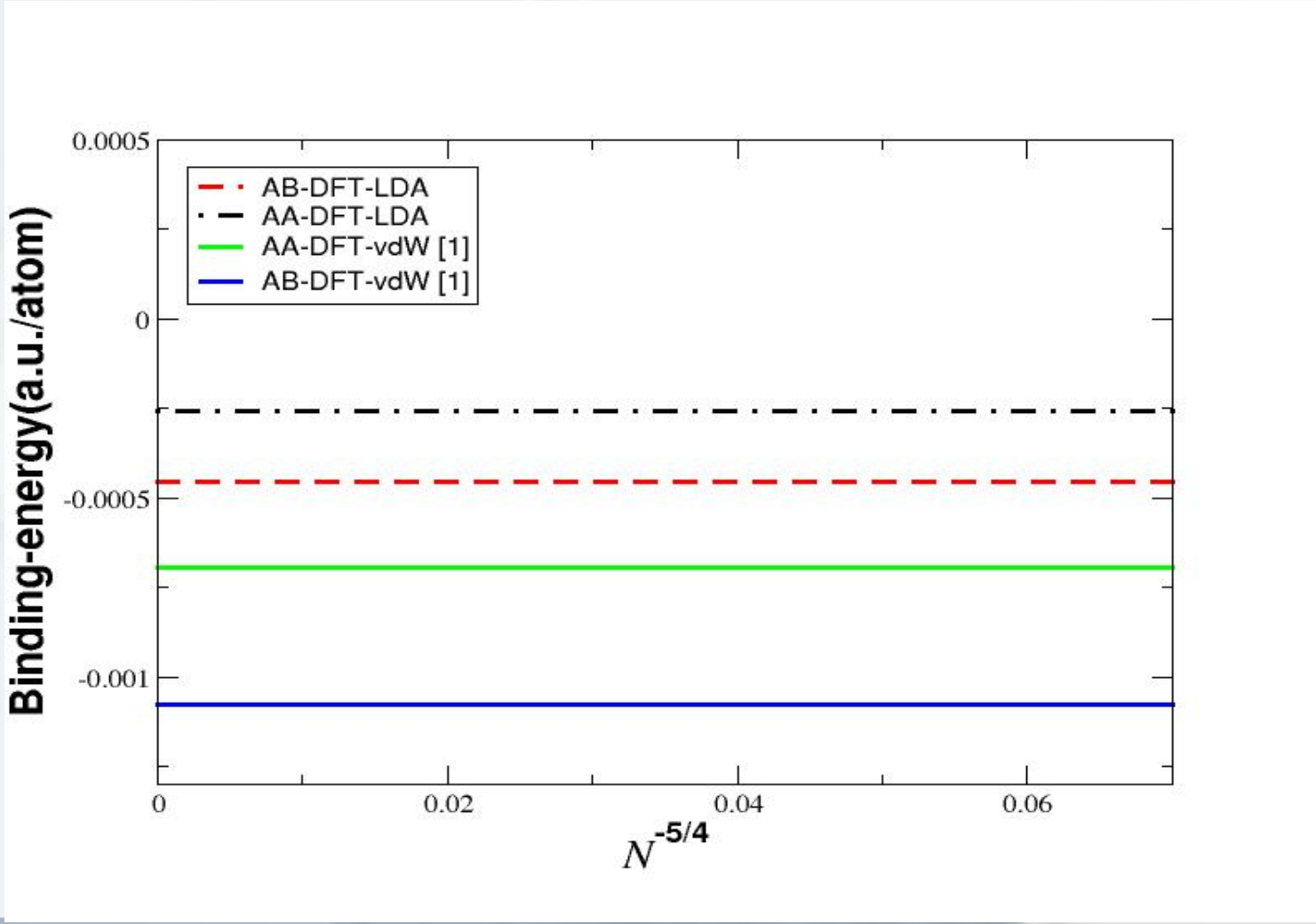
Bilayer zero energy:
0.0252 a.u./prim.cell

Share in BE: 10^{-6} a.u./prim.cell

Binding energy of bilayer

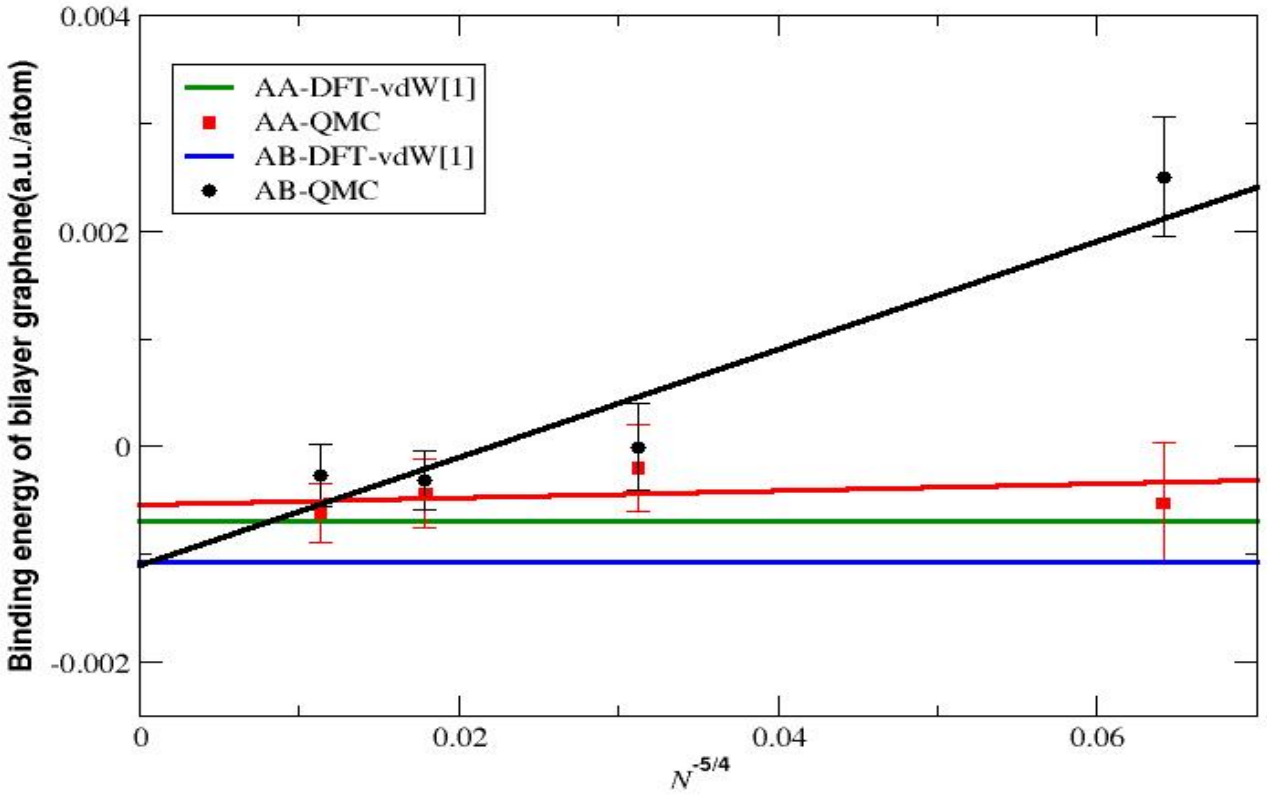


DFT calculations



1. I. V. Lebedeva et al., Phys. Chem. Chem. Phys. 13, 5687-5695 (2011).

Compare results



1. I. V. Lebedeva et al., Phys. Chem. Chem. Phys. 13, 5687-5695 (2011).

Summary

- Finite size error is a main limitation
- Not clear evidence if K vector offset is required for BE
- Binding energy of AB-stack larger (more stable) than AA-stack
- QMC calculation for AB-stack (33 meV/atom) in agreement with DFT-vdW (29 meV/atom)
- QMC calculation for AA-stack (12 mev/atom) smaller than DFT_vdW (19 mev/atom)

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Future work

- Reducing finite size errors by calculations for larger simulation cells
- Defining precise interlayer distance of graphene layers
- Binding energy of trilayer graphene in equilibrium interlayer distance
- Binding energy of graphene with other materials regarding to devices

Acknowledgment

Dr. Neil D. Drummond

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N8 Research Partnership


Thank you for your attention!