Exceptional service in the national interest

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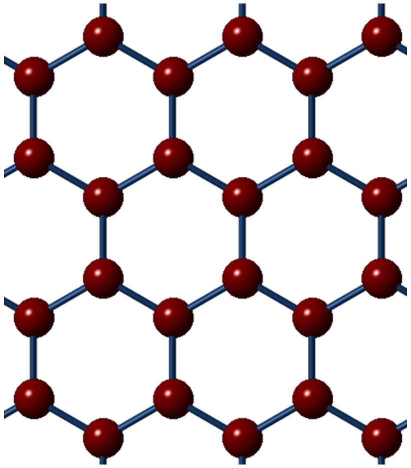

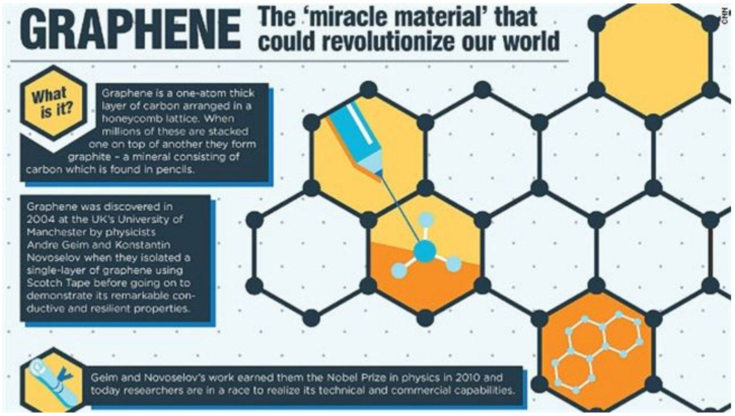

Graphene: the "Wonder" Material?

Hype vs. Realism: Using Materials Understanding to Filter BS

U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

Thomas Beechem

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Straw Poll

My familiarity with graphene is…..

1. Geim and Novoselov call me for advice
2. I use it
3. I've read about it
4. Is that the stuff that they make with Scotch tape?
5. Is it a new plotting app?

Text Questions: 505-933-1028

Learning Objectives

I want you to understand…

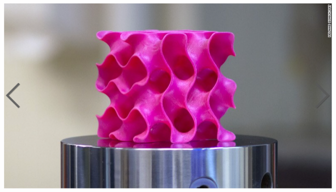
1. what graphene is and why everybody's excited
2. the origin of graphene's electrical, thermal, and optical properties
3. how to sift hype from reality for graphene and other wonder materials

Hype Train

CNN STYLE

Are we one step closer to being able to use the world's strongest material?

By Nicola Davison, CNN
Updated 8:33 AM ET, Fri January 13, 2017



Photos: Incredible innovations: These materials could change the world

Graphene-gyroid – Researchers at the Massachusetts Institute of Technology have designed a new material that is 10 times stronger than steel.

Recommended for you
Chicago judge killed outside home
Ex-MLB player Otis Nixon found safe

The Washington Post

Innovations

Why the graphene light bulb could switch on a new era of innovation

By Dominic Basulto April 2

Iron Man

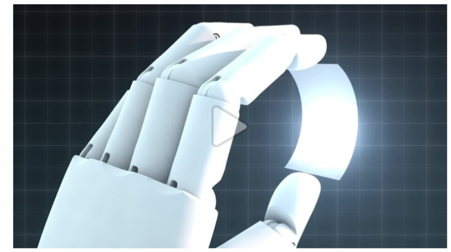
Why Iron man ditched iron for graphene

WIRED

CNN

Wonder material could harvest energy from thin air

By Peter Shadbolt, video produced by Curtis Brown and Jackson Loo, CNN
Updated 9:59 AM ET, Tue November 3, 2015



Top stories
News anchor learns her husband died in story she's reporting
Chicago judge killed outside home

Story highlights

- Researchers in the UK say a discovery involving wonder material graphene could revolutionize batteries
- Graphene is 200 times stronger than steel and a million times thinner than a human hair
- The material, which has the same atomic structure as the lead in pencils, is impermeable to atoms and molecules
- Scientists found that positively charged hydrogen atoms could pass through it with implications for fuel cell efficiency

Editor's Note: Originally published December 2014, updated November 2, 2015.

(CNN) — Bold claims for new battery technology have been around since the invention of the lead-acid battery more than 150 years ago.

But researchers at Manchester University in the UK say their latest discovery involving the new wonder material graphene could be the most revolutionary advance in battery technology yet.

According to a study published in the journal Nature,

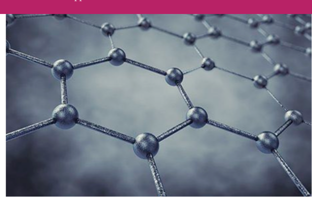
theguardian

Physics

Graphene - the new wonder material

Scientific interest rolls in for a material that is more solid than steel and a better conductor than copper

David Larousserie
Friday 22 November 2013 11.01 EST



3D illustration showing a sheet of graphene. Photograph: nobeastsofierce/Alamy

The molecule is priceless but it is not a matter of cost - a few hundred dollars per kilo. The value lies in its potential. The molecule in question is called graphene and the EU is prepared to devote €1bn ($1.3bn) to it between 2013 and 2023 to find out if it can transform a range of sectors such as electronics, energy, health and construction. According to Scopus, the bibliographic database, more than 8,000 papers have been written about graphene since 2005.

Most popular in US
British spies were first to spot Trump team's links with Russia
Arizona Sky Village's residents have one rule: 'Turn off your goddamned lights'
United States' first female Muslim judge, Sheila Abdus-Salaam, found dead in New York

Bits — The New York Times

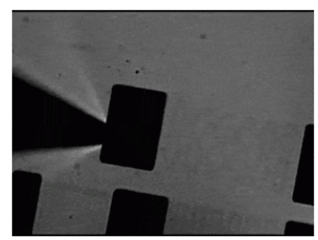
Graphene Could Usher in Flexible, Ultra-Slim Gadgets

By NICK BILTON OCTOBER 12, 2012 5:54 PM

You've probably never heard of graphene, a carbon-based material, but it might be stuffed into your pocket or wrapped around your wrist in the not-too-distant future.

Graphene is a fully flexible material. Ji Hye Hong

According to the



Graphene can be folded and cut into a microscopic kirigami spring.
Cornell University/McEuen Group

The New York Times

JULY 30, 2015

Graphene Origami

Graphene is a thin material with tremendous potential. Measuring only an atom-thick, it is harder than diamond, a better electrical conductor than copper, and 200 times as strong as steel.

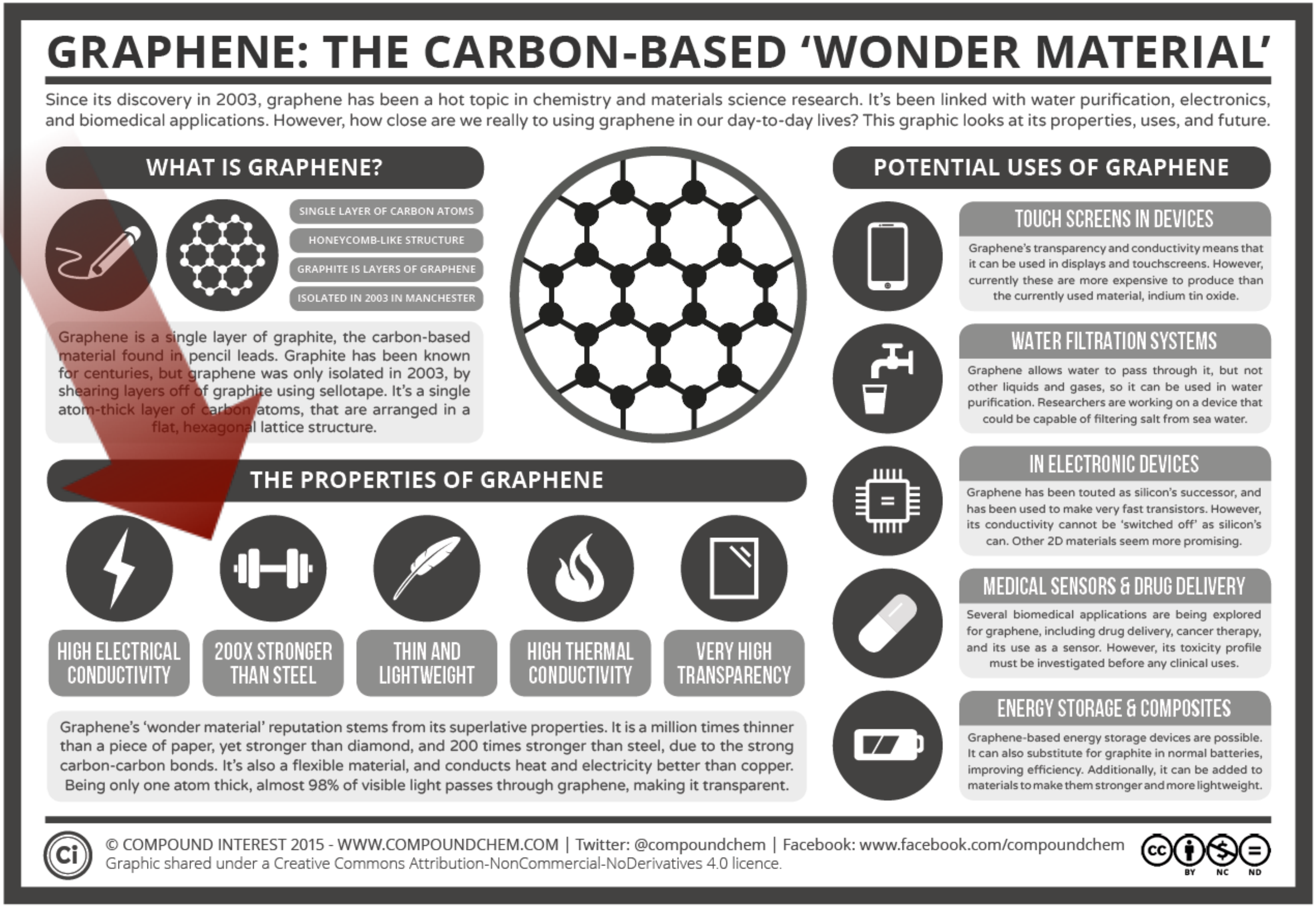
Graphene is so strong that a sheet of it stretched across a coffee-cup should be able to support the weight of a truck bearing down on a pencil point. Some researchers call it a "wonder material" that could be used in everything from batteries and biosensors to computers and condoms.

Now researchers have discovered another one of graphene's feats: It's as flexible as paper. Not only can graphene be crumpled and then perfectly flattened, but it can also be folded like origami, according to a report published Wednesday in Nature.

Using a style of origami that involves cuts and folds called kirigami, the researchers fashioned a sheet of graphene into a tiny spring. According to Nature, researchers may one day use kirigami to craft graphene sheets into microscopic weighing scales or nets small enough to wrap around living cells.

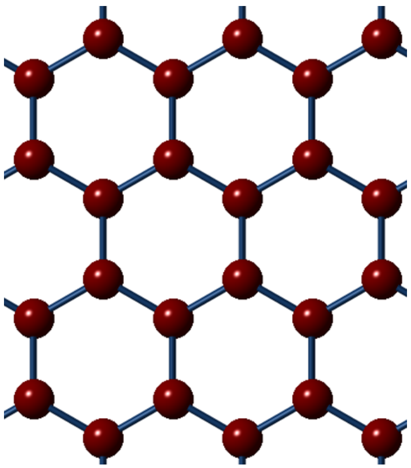
—NICHOLAS ST. FLEUR

Wonder Material Properties

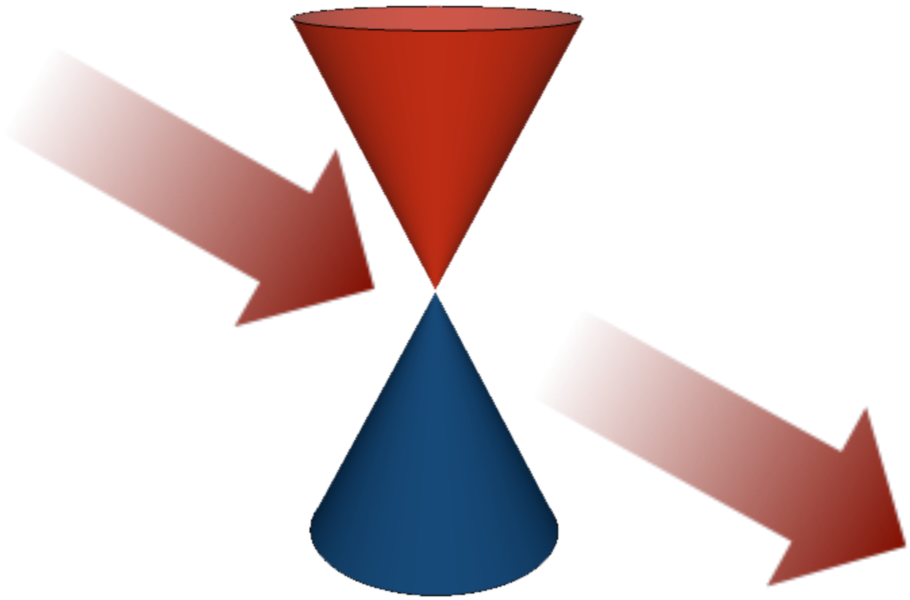


Origin: Properties

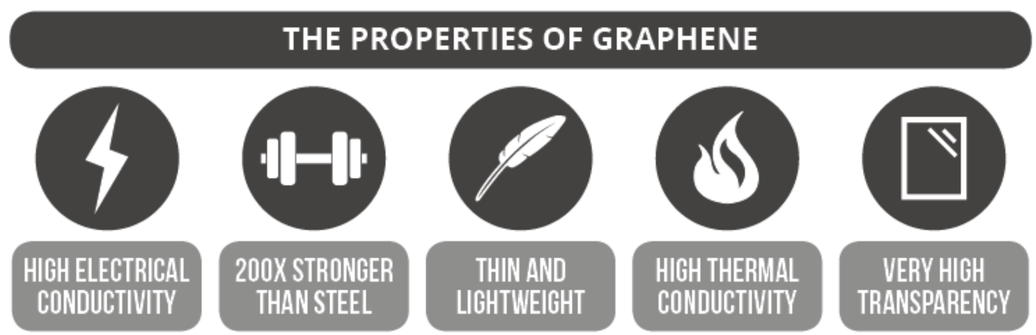
Periodicity



Bandstructure



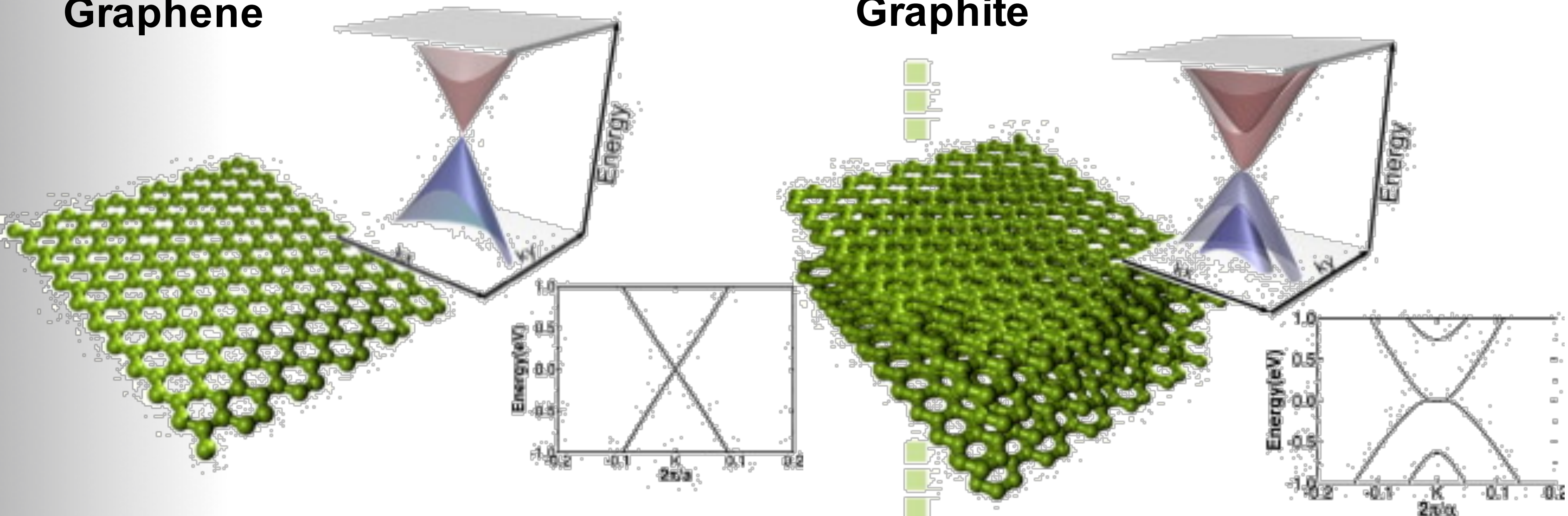
Properties



Question:
What's so novel about graphene's periodicity?

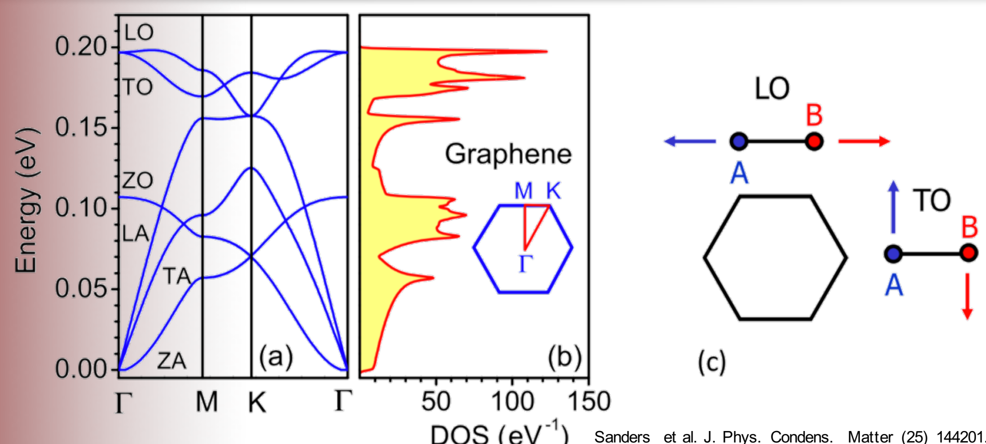
Electronic & Lattice Bandstructure

Electronic

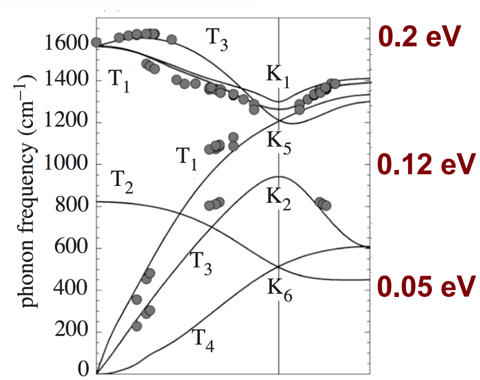


Terrones et al. nanotoday (5) 351, 2010.

Lattice



Sanders et al. J. Phys. Condens. Matter (25) 144201. 2013



Reich and Thomson. Phil. Trans. R. Soc. Lond. A (362) 2271. 2014

Question: When does "multilayer" graphene turn into graphite?

Counting Carriers

PREMISE: Amount of energy (electric, heat, optical) moved proportional to the number of energy carriers.

Question: How many carriers does graphene have?

Number of Charge Carriers

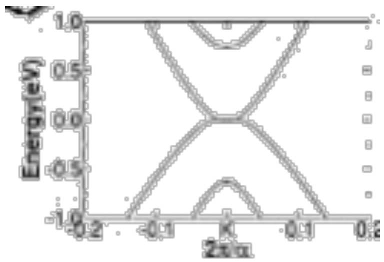
$$n = \int D(E) f_f(E) dE$$

3D

$$D(k) = 2\frac{4\pi k^2 dk}{(2\pi/L)^3 V} = \frac{k^2 dk}{\pi^2}$$

Parabolic Dispersion

$$E - E_c = \frac{\hbar^2 k^2}{2m^*}$$



3D-DOS (Volumetric)

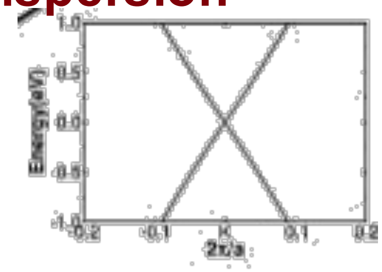
$$D(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E - E_c}$$

2D

$$D(k) = 4\frac{(2\pi k)dk}{(2\pi/L)^2 A} = \frac{2k\, dk}{\pi}$$

Linear Dispersion

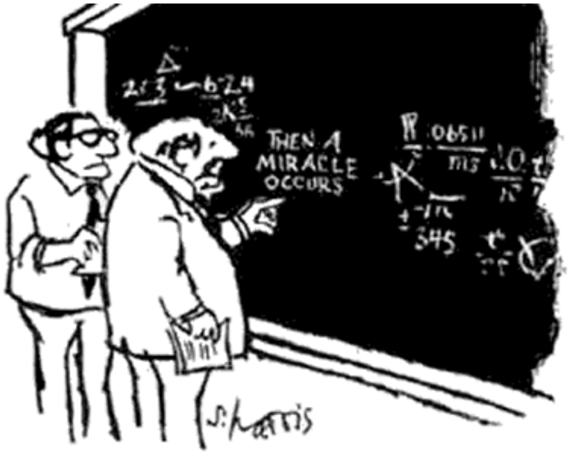
$$E - E_c = \hbar v_f k$$



2D-Linear-DOS (Areal)

$$D(E) = \frac{2(E - E_c)dE}{\pi(\hbar v_f)^2}$$

Number of Charge Carriers



"I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO."

$$n = \int D(E) f_f(E) dE$$

3D-Parabolic

$$n = N_c F_{1/2}\left(-\frac{E_c - E_f}{k_B T}\right)$$

$$N_c = 2\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)^{3/2}$$

2D-Linear

$$n = N_{c,g} F_1\left(-\frac{E_c - E_f}{k_B T}\right)$$

$$N_{c,g} = \left(\frac{2^{1/2} k_B T}{\pi^{1/2}\hbar v_f}\right)^2$$

Challenge: How does the number of carriers compare in graphene vs. traditional semiconductors?

Team Silicon
Bandgap= 1.1eV
Effective mass=1.08 m_0

Team Graphite
Bandgap= 0 eV
Effective mass=0.043 m_0

Team Graphene
Bandgap= 0 eV
Effective mass=0 m_0

Dora's Backpack

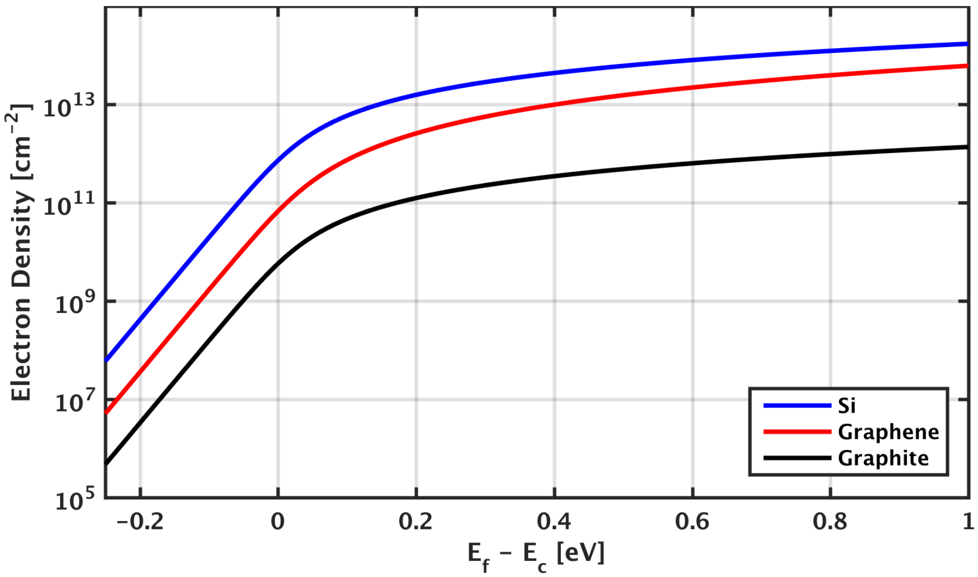
Thickness of Si and Graphite is 0.335 nm

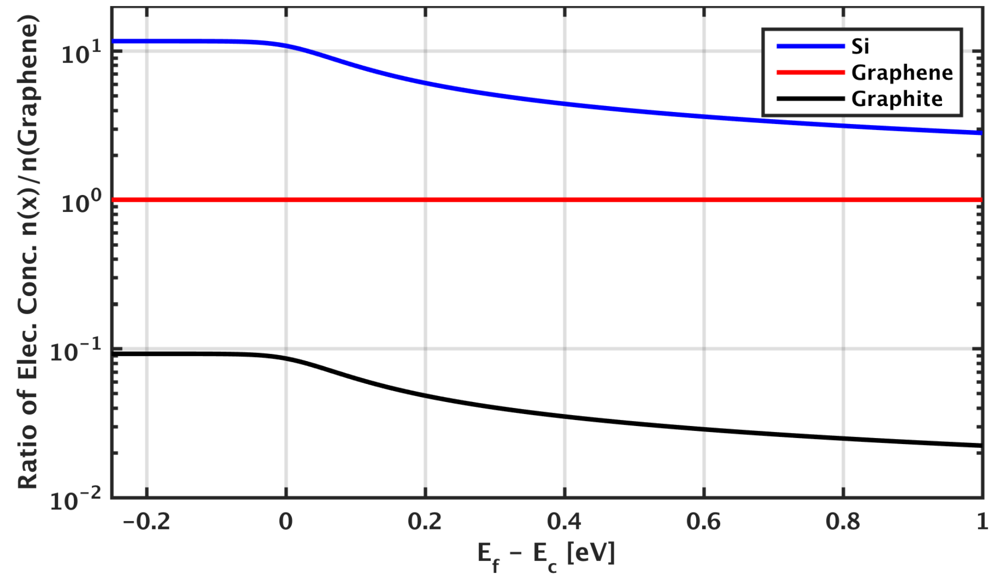
Assume Fermi-level starts at -0.2 eV below Ec and goes to 0.75 eV

Temperature= 4, 77, and 300K

\hbar=1.054e-34 J-s
K_b=1.380e-23 J/K
m_o=9.109e-31 Kg
v_f=1e6 m/s

Number of Charge Carriers



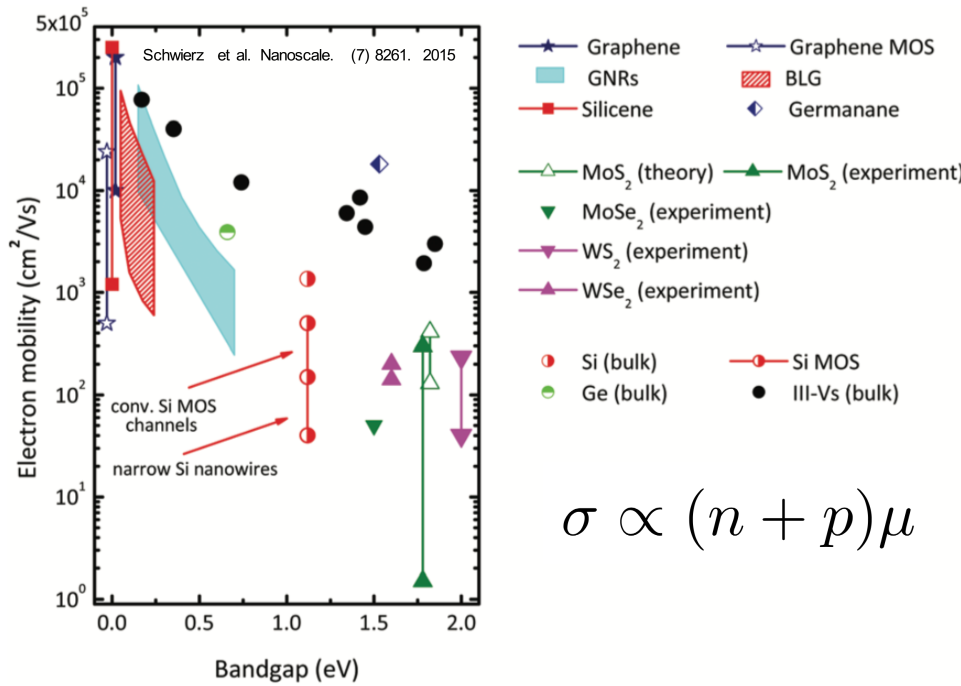


Good News

- Lower electron concentration
- High electron mobility
- High hole mobility

Bad News

- Lower electron concentration
- High mobility <u>SOMETIMES</u>
- See above



$$\sigma \propto (n+p)\mu$$

Electrical: Is graphene good for this?

Critical Questions

1. What mobility do I need for it to work?
2. Is it an intensive or extensive application?
3. Does graphene offer something ”else” that I can’t get otherwise?

Learning Objectives

Sandia National Laboratories

I want you to understand...

1. what graphene is and why everybody's excited
2. the origin of graphene's electrical, thermal, and optical properties
3. how to sift hype from reality for graphene and other wonder materials

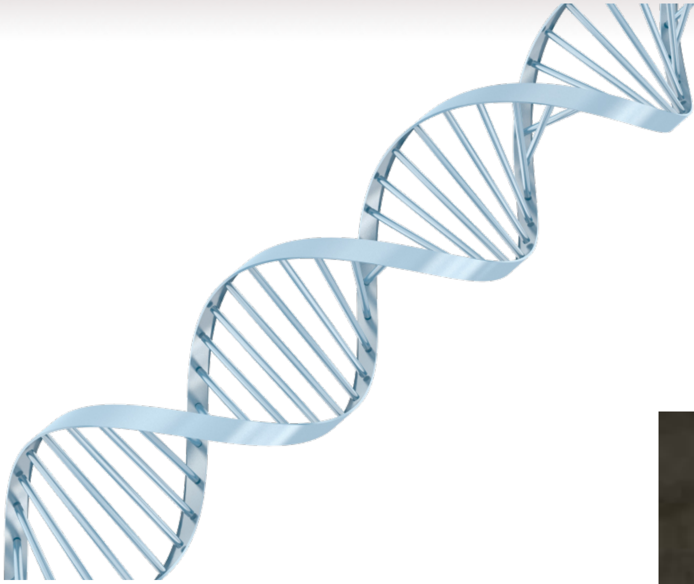
Key Takeaways thus far

1. Periodicity, Bandstructure Property
2. Difference between graphene and graphite
3. Graphene Bandstructure: 2D-DOS & Linear Bands

What makes me, me?

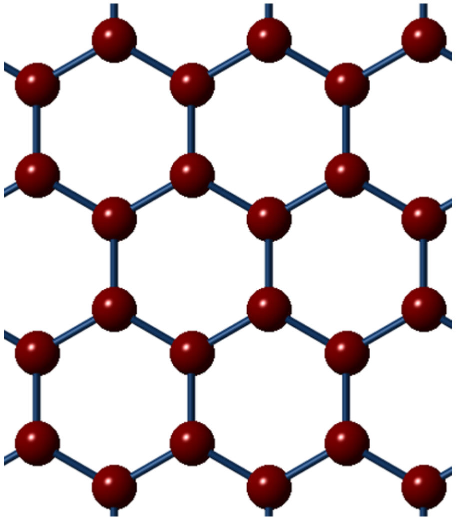
Genetic, Intrinsic

Environment

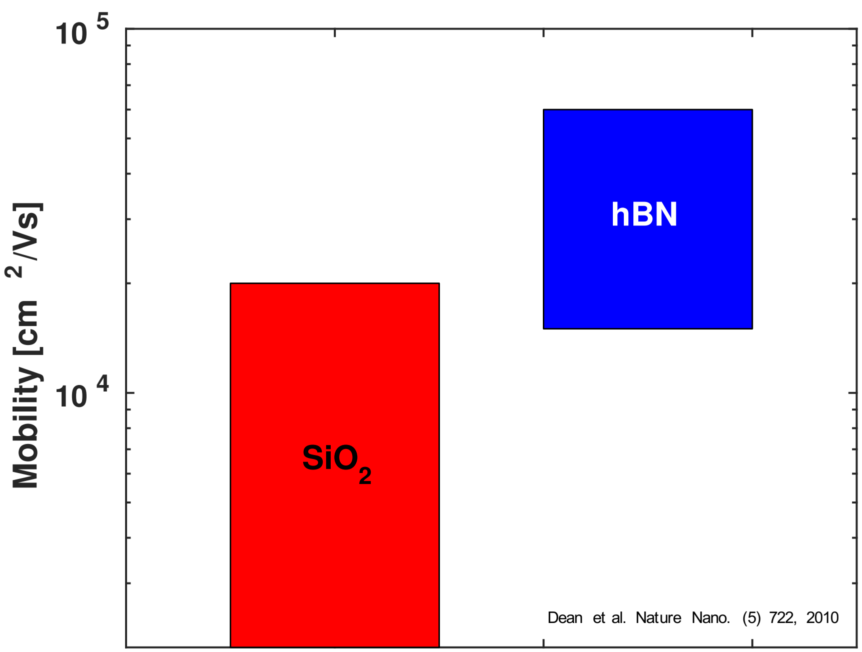


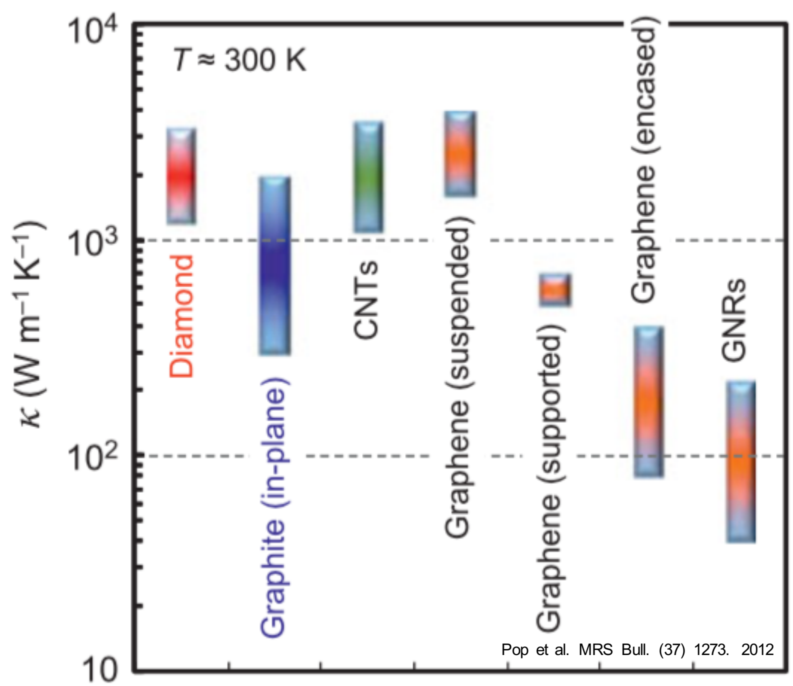
Takeaway: We are who we are AND what we're around.

Env.:Graphene & Peer Pressure



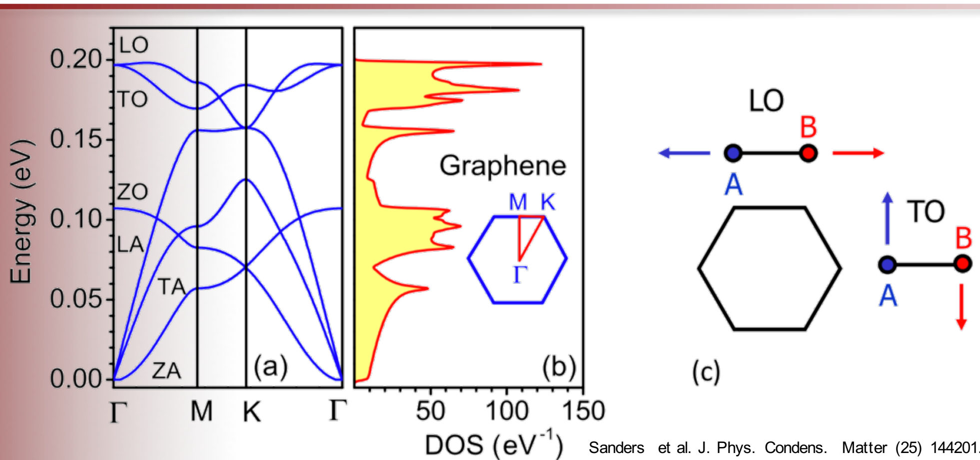
D.A.R.E.®



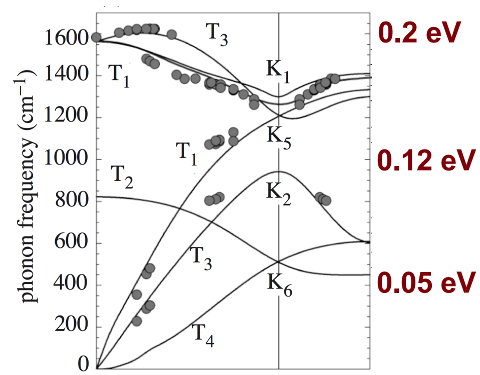


Lattice Bandstructure: Thermal

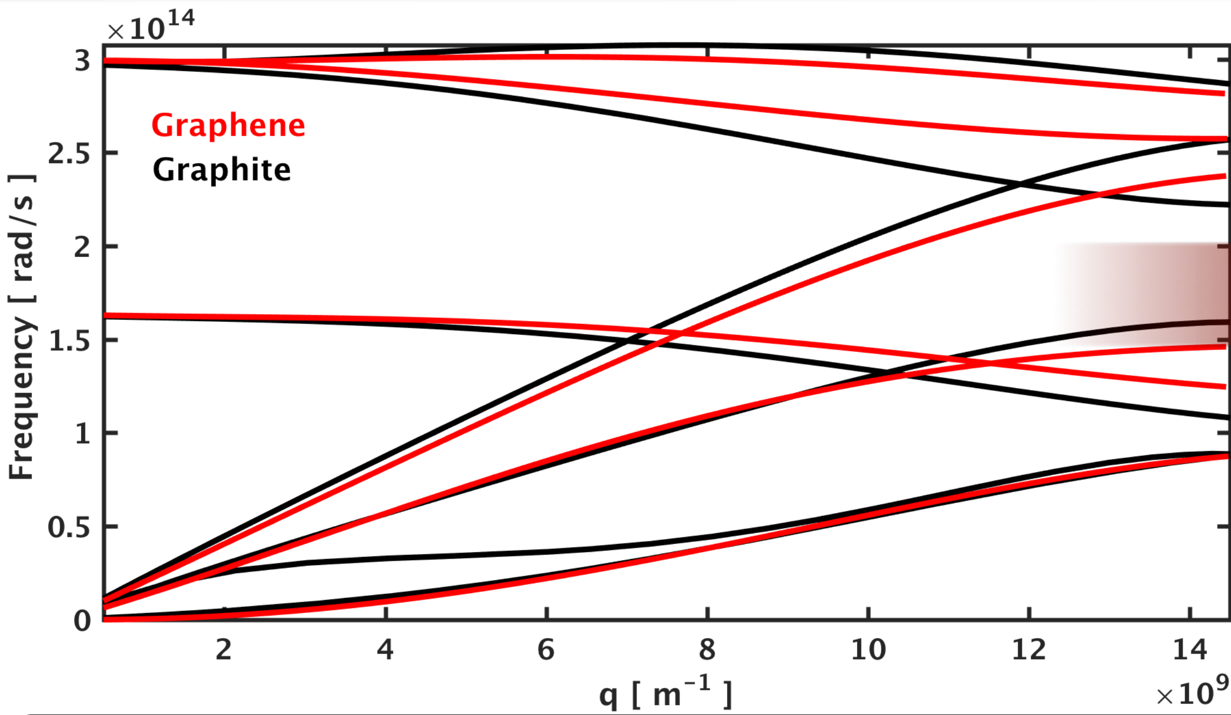
Lattice



Sanders et al. J. Phys. Condens. Matter (25) 144201. 2013



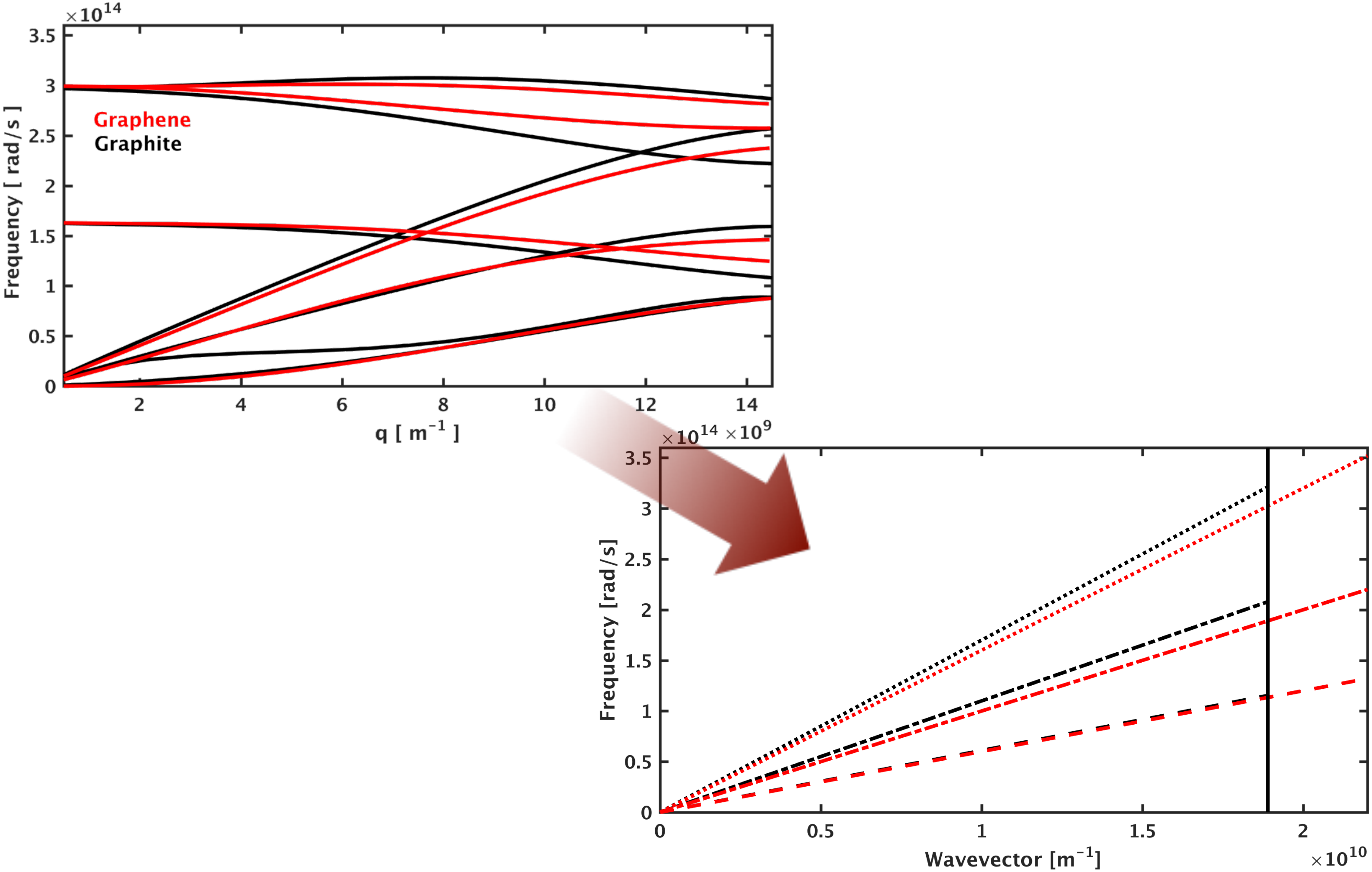
Reich and Thomson. Phil. Trans. R. Soc. Lond. A (362) 2271. 2014



$$k = \sum_i C_i v_i \Lambda_i$$

Question: Why is graphene's thermal conductivity sometimes more & sometimes less than graphite?

Number of Heat Carriers: Debye



Number of Heat Carriers

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$$n = \sum_{i}^{3} \int_{0}^{\omega_{i,max}} D(\omega) f_{BE}(\omega) d\omega$$

3D

$$D(k) = \frac{4\pi k^2 dk}{(2\pi/L)^3 V} = \frac{k^2 dk}{2\pi^2}$$

3D-Debye

$$\omega = v_i k$$

3D-DOS (Volumetric)

$$D(\omega) = \frac{\omega^2 d\omega}{v_i^3 \pi^2}$$

Max. Frequency

$$\omega_{i,max} = v_i k_{max}$$

Max. Wavevector

$$q_{max} = \left(6\pi^2 n_o\right)^{1/3}$$

2D

$$D(k) = \frac{2\pi k dk}{(2\pi/L)^2 A} = \frac{k dk}{2\pi}$$

2D-Debye

$$\omega = v_i k$$

2D-DOS (Areal)

$$D(\omega) = \frac{\omega d\omega}{v_i^2 2\pi}$$

Max. Frequency

$$\omega_{i,max} = v_i k_{max}$$

Max. Wavevector

$$q_{max} = \left(4\pi n_o^*\right)^{1/2}$$

Number of Heat Carriers

Sandia National Laboratories

Challenge: How many phonons exist in each Debye branch for graphene and graphite

Parameter	Graphene	Graphite
n_0 [atoms/cm$^{2(3)}$]	3.85e15	1.14e23
v_1 [Km/s]	16	17
v_2 [Km/s]	10	11
v_3 [Km/s]	6	6

$$n = \sum_i^3 \int_0^{\omega_{i,max}} D(\omega) f_{BE}(\omega) d\omega$$

3D

$$D(k) = \frac{4\pi k^2 dk}{(2\pi/L)^3 V} = \frac{k^2 dk}{2\pi^2}$$

3D-Debye

$$\omega = v_i k$$

3D-DOS (Volumetric)

$$D(\omega) = \frac{\omega^2 d\omega}{v_i^3 \pi^2}$$

Max. Frequency

$$\omega_{i,max} = v_i k_{max}$$

Max. Wavevector

$$q_{max} = \left(6\pi^2 n_o\right)^{1/3}$$

2D

$$D(k) = \frac{2\pi k dk}{(2\pi/L)^2 A} = \frac{k dk}{2\pi}$$

2D-Debye

$$\omega = v_i k$$

2D-DOS (Areal)

$$D(\omega) = \frac{\omega d\omega}{v_i^2 2\pi}$$

Max. Frequency

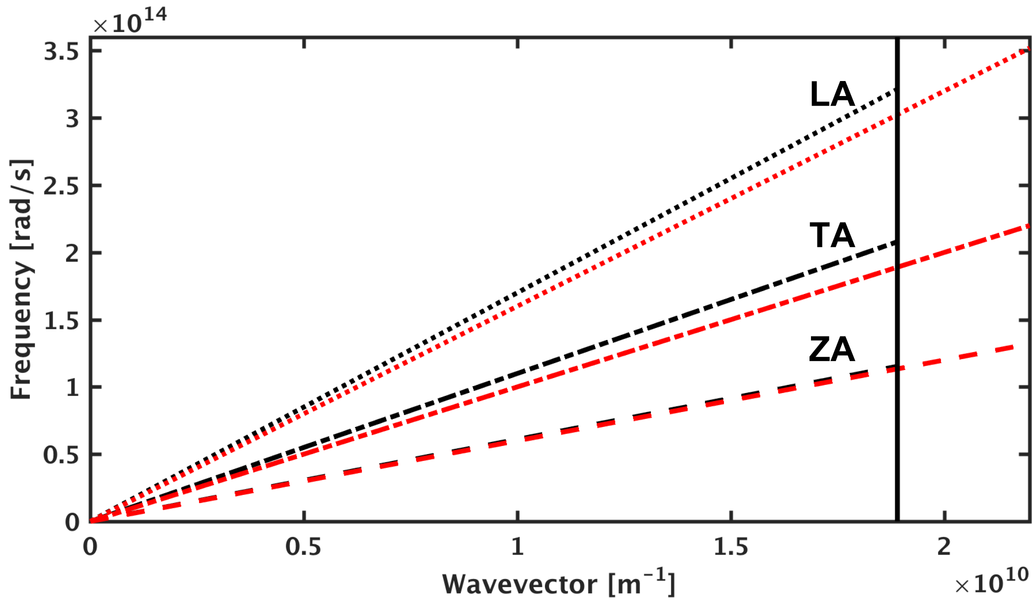
$$\omega_{i,max} = v_i k_{max}$$

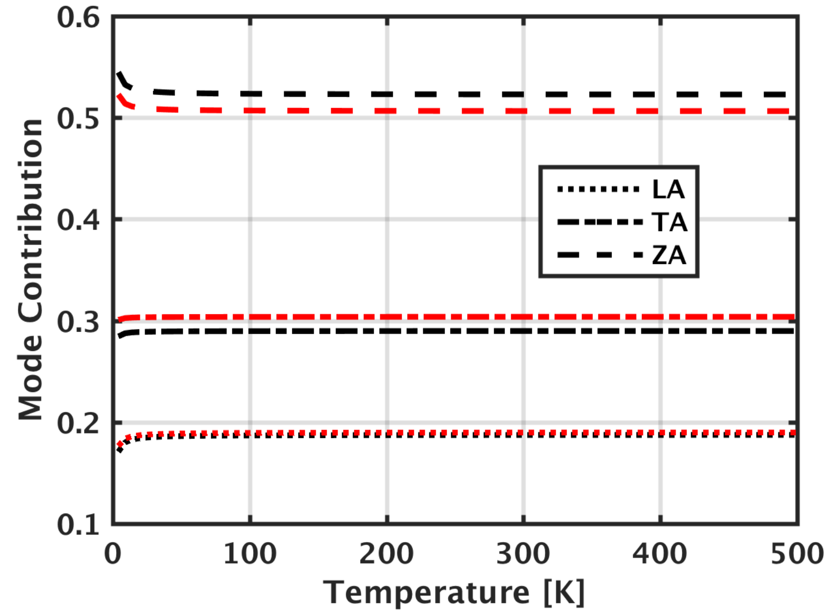
Max. Wavevector

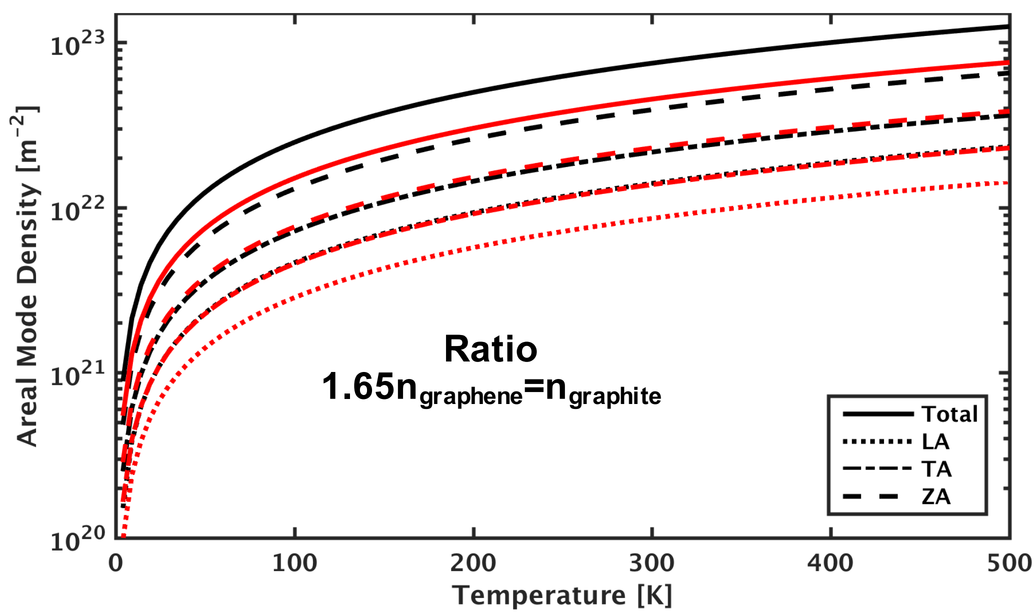
$$q_{max} = (4\pi n_o^*)^{1/2}$$

Challenge: What happens if you remove the v_3 branch in graphene?

Number of Heat Carriers

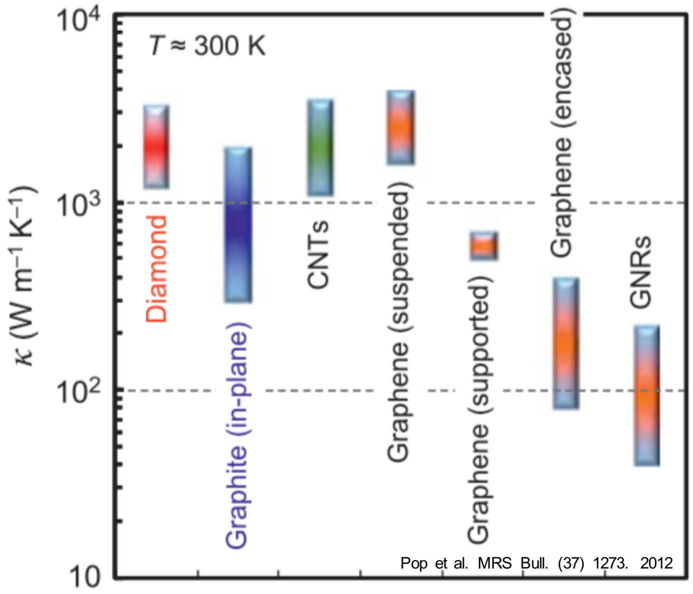


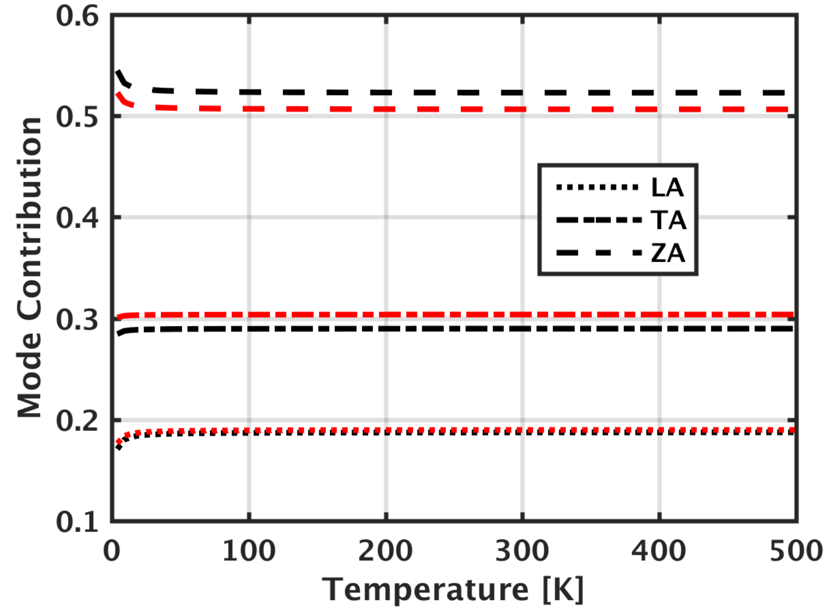


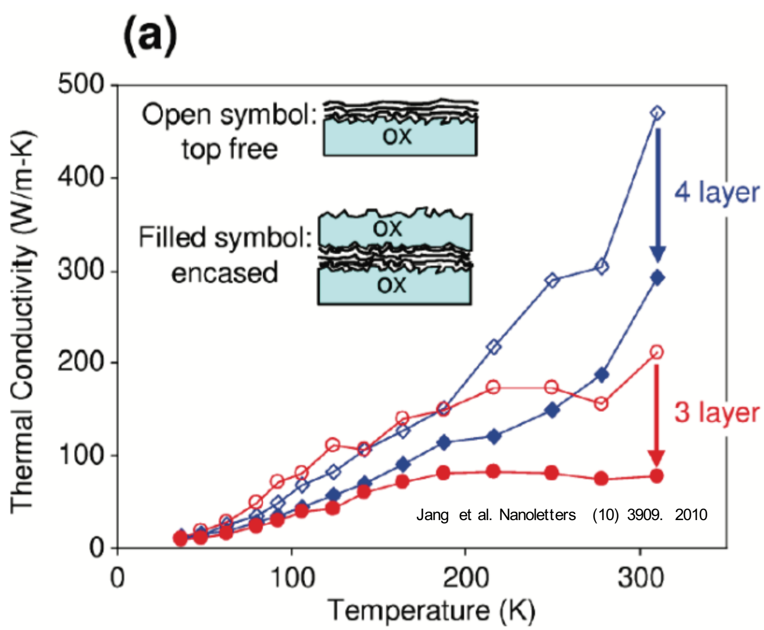


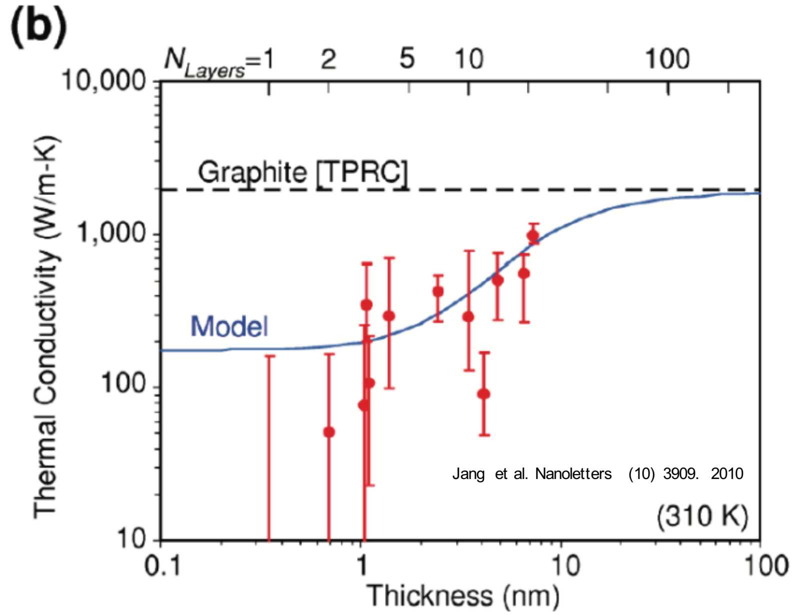
Question:
Out of plane mode is biggest contributor. Is that bad?

Thermal Properties









Thermal: Is graphene good for this?

Critical Questions

1. Is the graphene touching anything?
2. Is it an intensive or extensive application?
3. No…Just No....It's not a thermal solution.

Learning Objectives

I want you to understand...

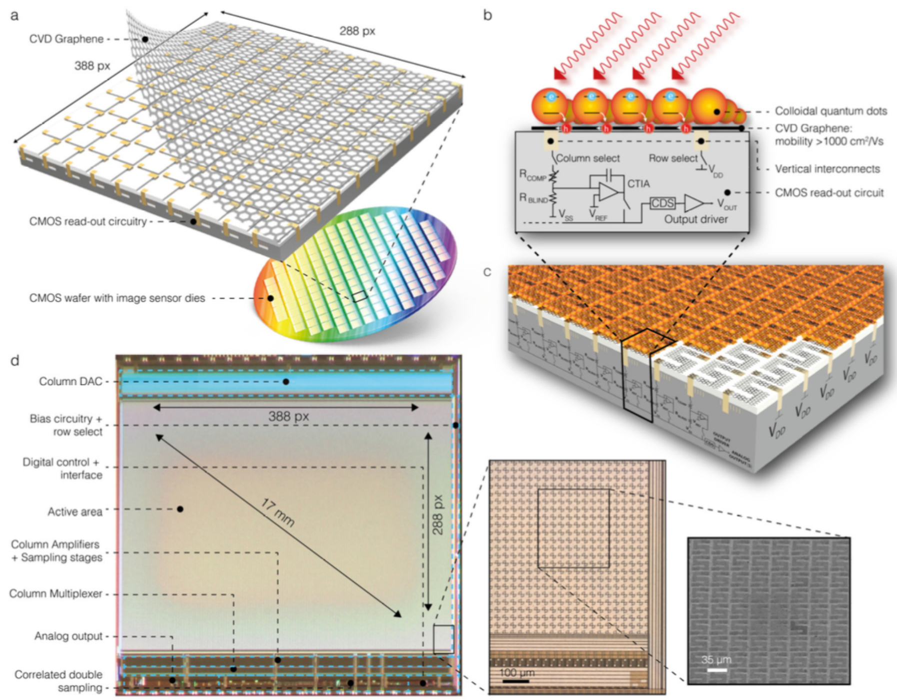
1. what graphene is and why everybody's excited
2. the origin of graphene's electrical, thermal, and optical properties
3. how to sift hype from reality for graphene and other wonder materials

Key Takeaways thus far

1. Periodicity, Bandstructure Property
2. Difference between graphene and graphite
3. Bandstructure: 2D-DOS & Linear Bands
4. Bandstructure: Debye Solid & the impact of ZA
5. Impact of surroundings on properties

Can Graphene See?

Graphene Digital Camera



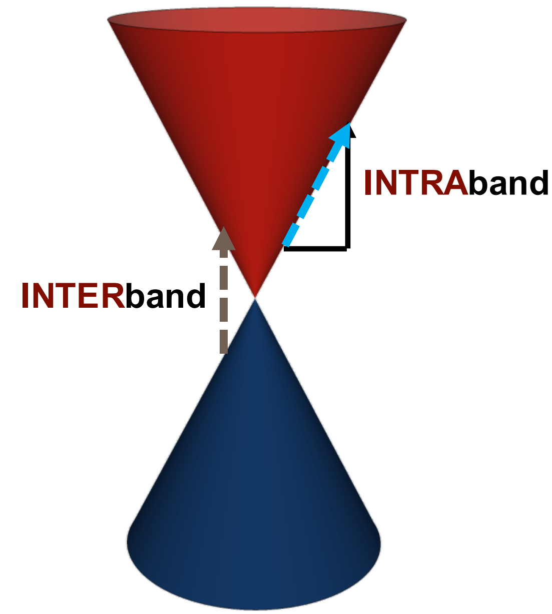
Goosens et al. Arxiv 1701.03242 2017

Question: Why is graphene a promising optical material?

Optical: Controlling Transitions

Sandia National Laboratories

PREMISE: Must conserve energy and momentum to create an optical transition

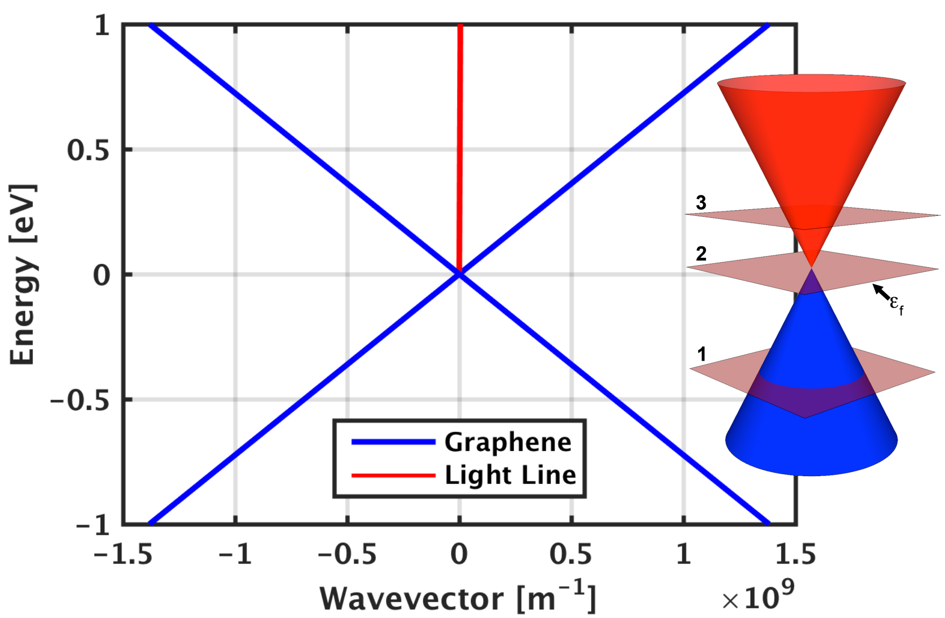


Graphene Dispersion

$$E - E_c = \hbar v_f k$$

Photon Dispersion

$$E = \hbar c k = \frac{hc}{\lambda}$$

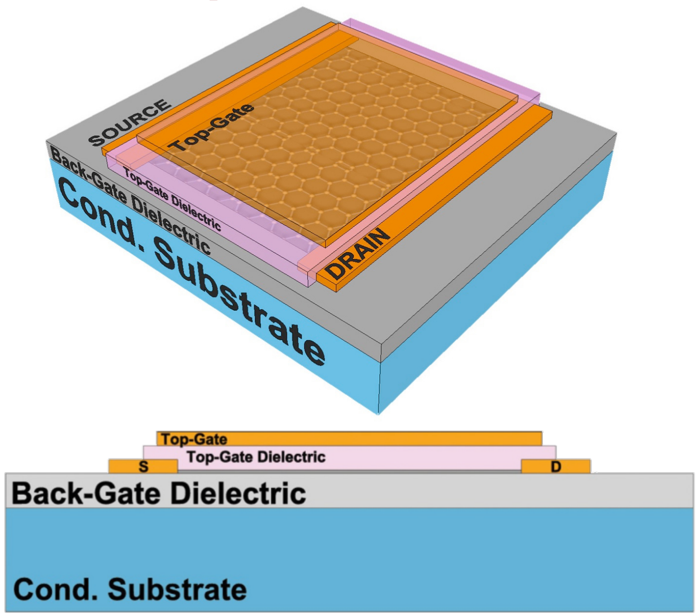


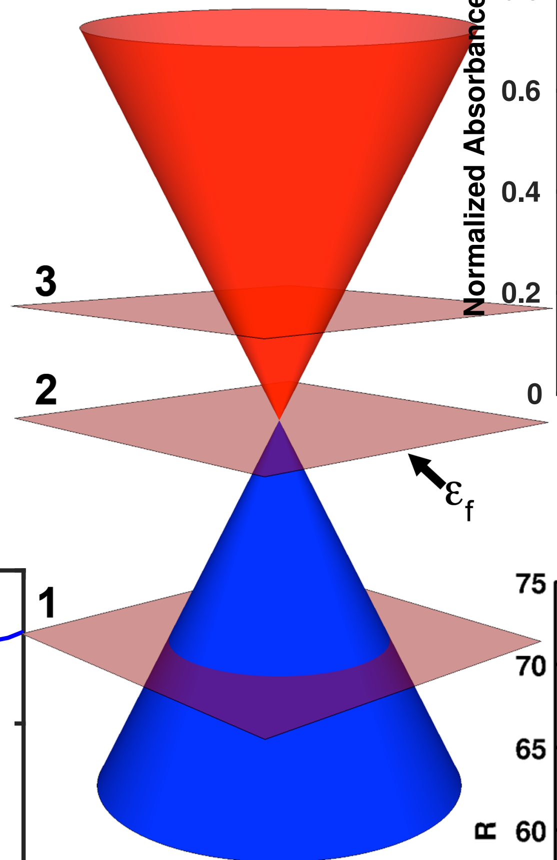
Question:
What happens when Fermi-level changes?

Optical: Controlling Transitions

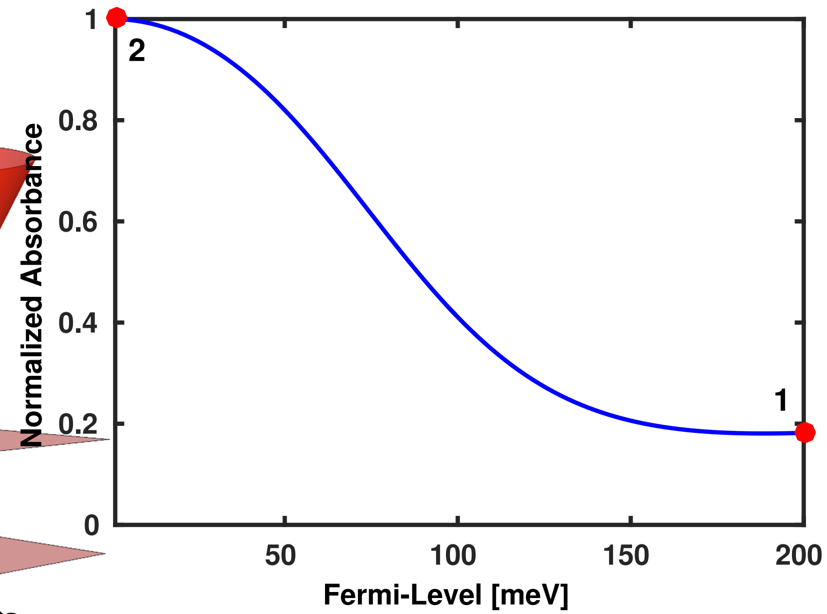
Sandia National Laboratories

Graphene Transistor

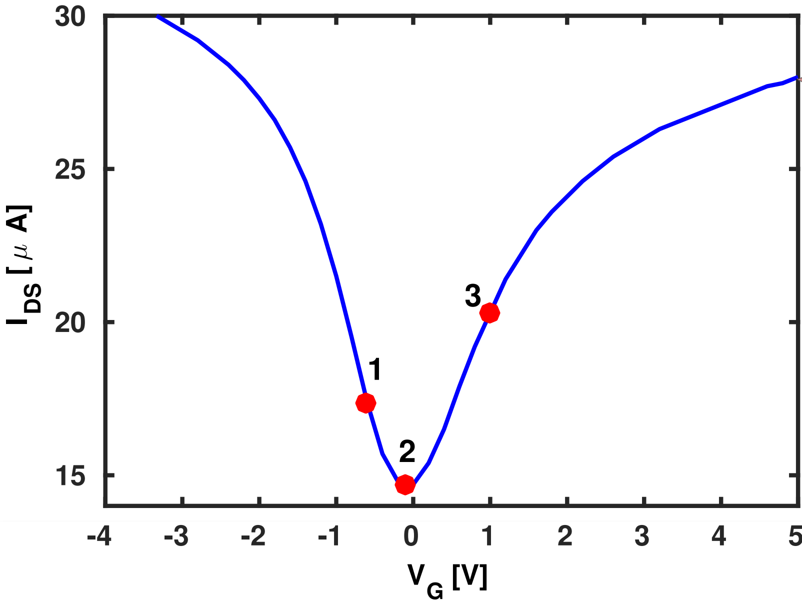




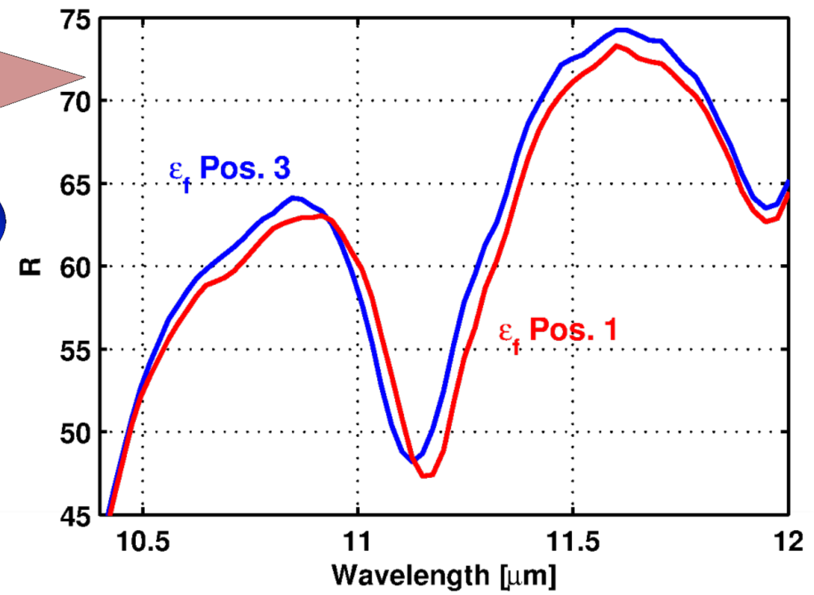
Tunable Absorber



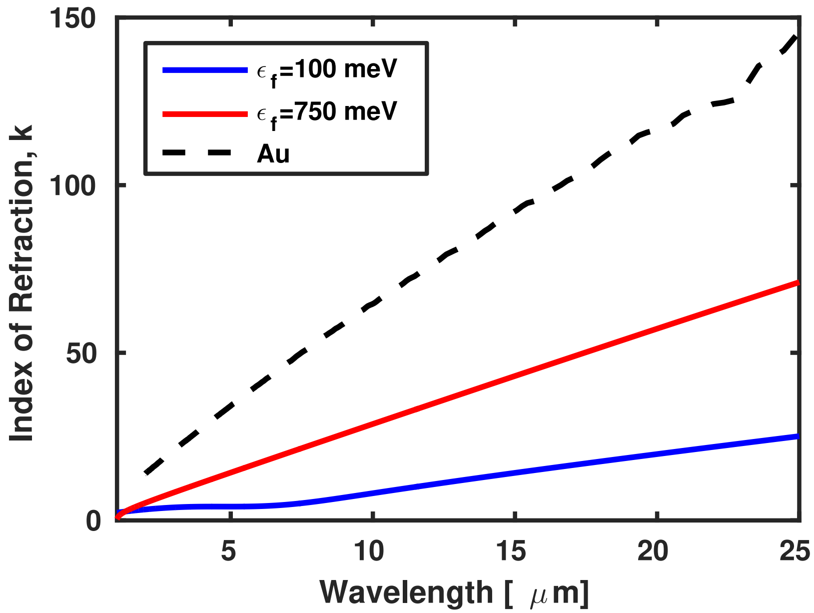
Tunable Resistance

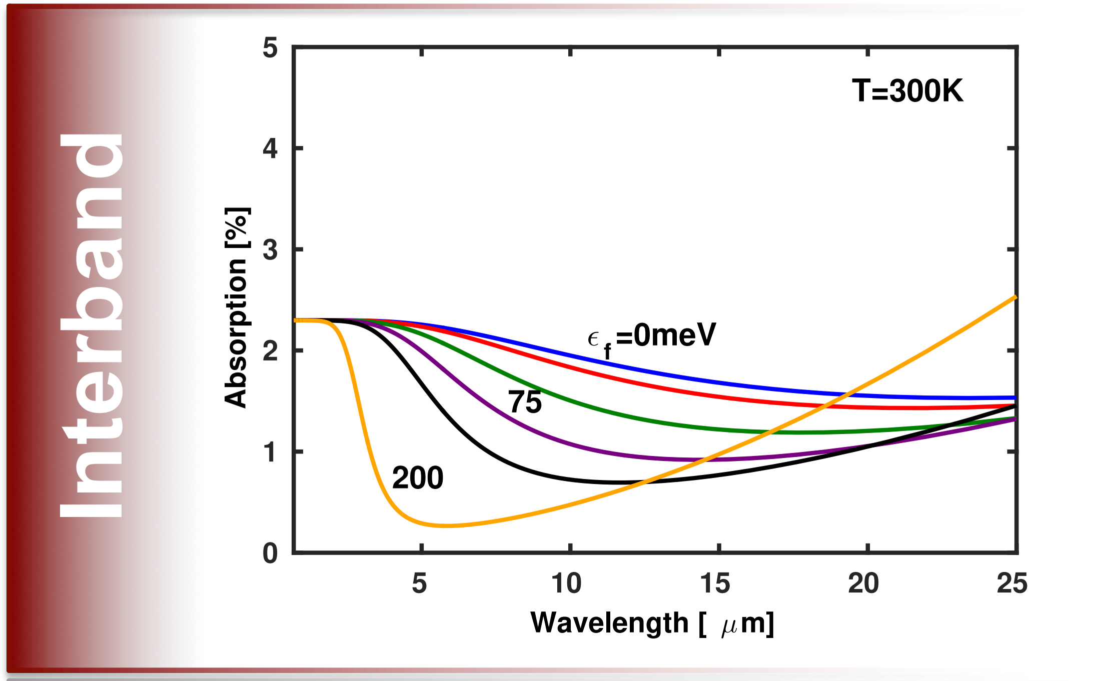


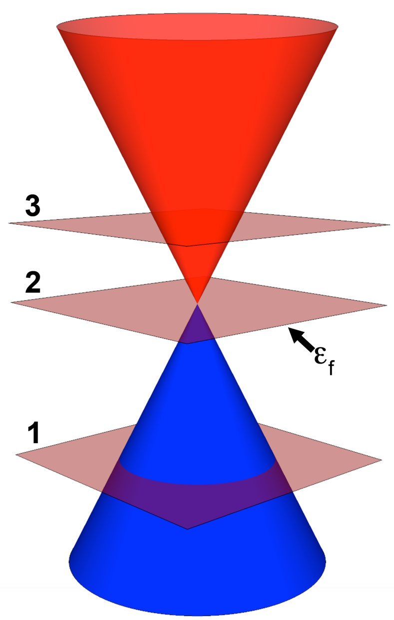
Tunable Nanoantenna

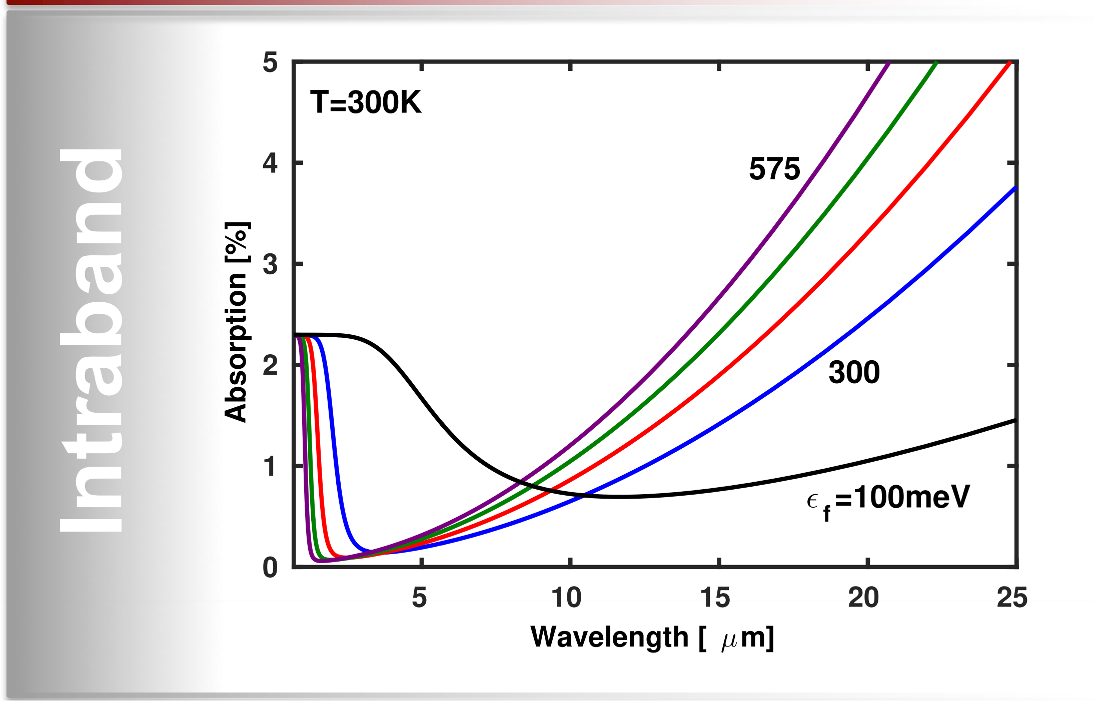


Myth: Graphene Absorbs 2.3%









Optical Counting Transitions

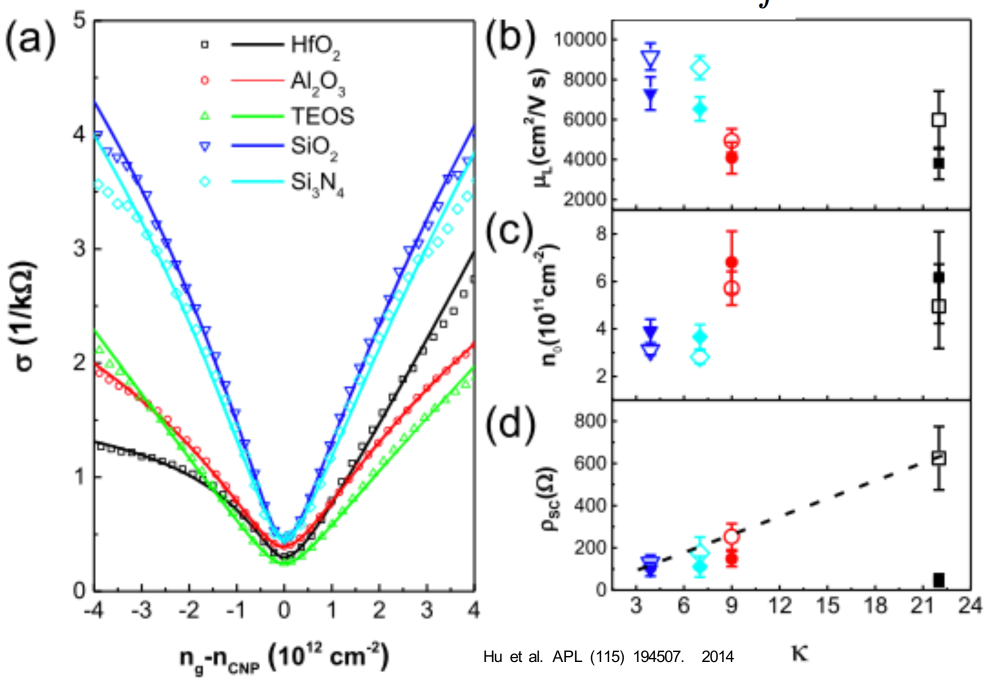
Challenge: How much charge can I have & still absorb 500 nm, 1 μm, 10 μm?

"Absorbable" Light

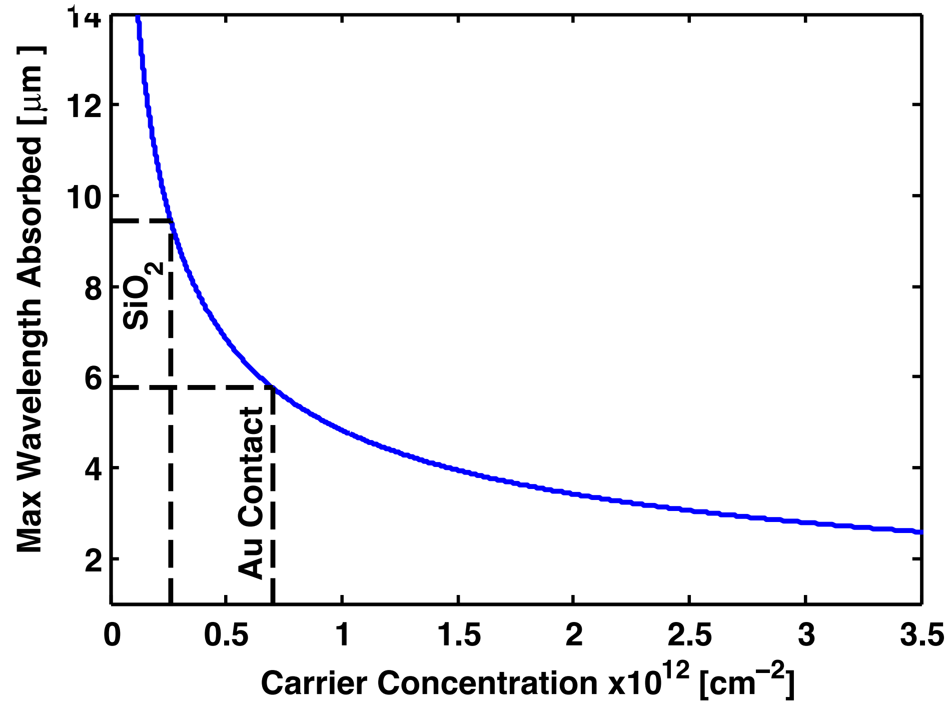
$$\lambda_{max} = \frac{hc}{2\epsilon_f}$$

Fermi-Level & Charge

$$\epsilon_f = \frac{hv_f}{2\pi}\sqrt{\pi n}$$

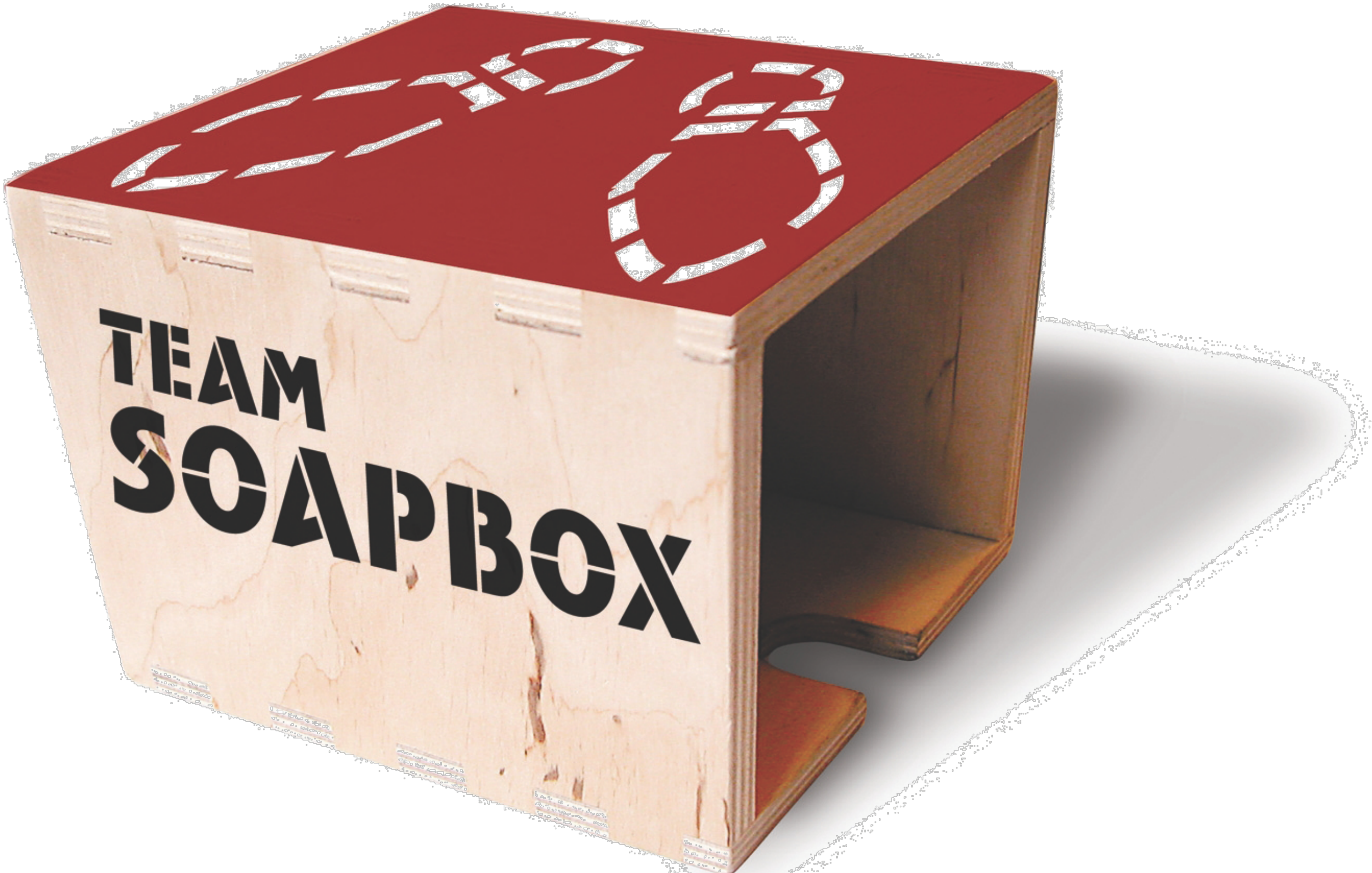


Hu et al. APL (115) 194507. 2014



Takeaway: You don't get all your Fermi-levels in real life.

Optical: Is graphene good for this?



Critical Questions

1. Does the wavelength match my Fermi-levels?
2. How much absorption do I really need?
3. Can another material do the same thing?

Learning Objectives

I want you to understand…

1. what graphene is and why everybody's excited
2. the origin of graphene's electrical, thermal, and optical properties
3. how to sift hype from reality for graphene and other wonder materials

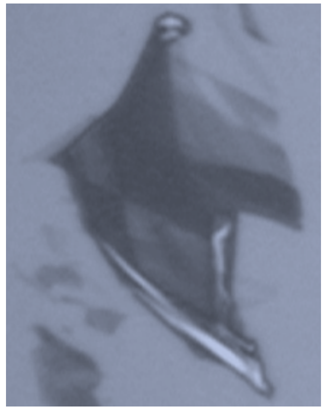
Key Takeaways

1. Periodicity, Bandstructure Property
2. Difference between graphene and graphite
3. Bandstructure: 2D-DOS & Linear Bands
4. Bandstructure: Debye Solid & the impact of ZA
5. Impact of surroundings on properties
6. Differentiation from other materials

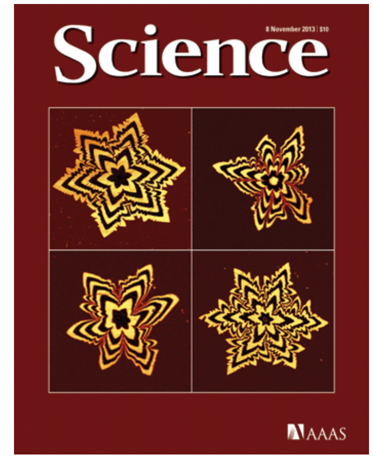
``Brands” of Graphene

Sandia National Laboratories

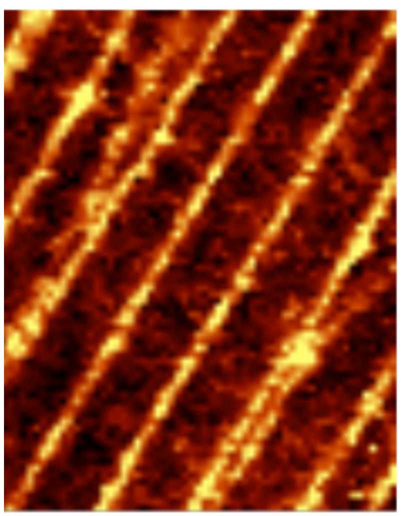
Exfoliated

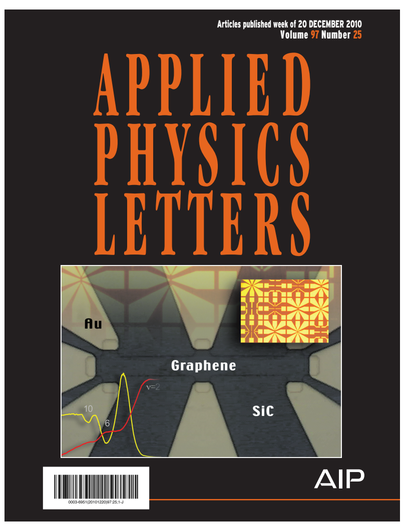


Copper Based CVD

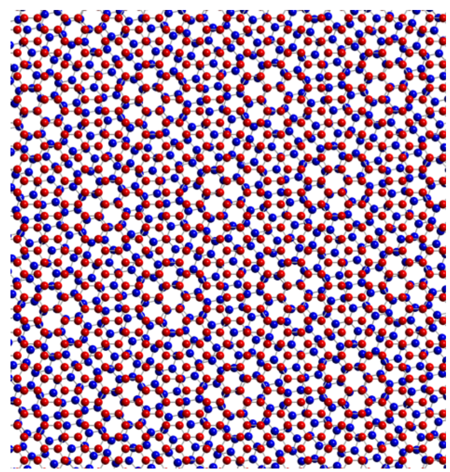


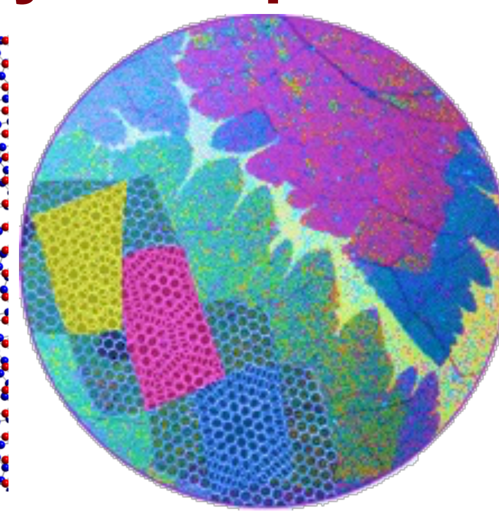
Epitaxial on SiC





Twisted Bilayer Graphene





Epi: Pan, Howell, Ohta, et al. APL (97) 252101. 2010.

CVD: Hao et al. Sci. (342) 720, 2013.