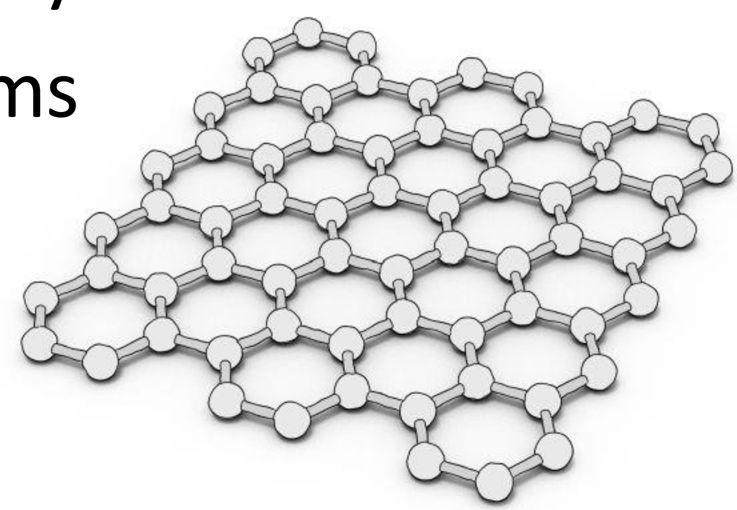
Graphene: Electronic and vibrational properties

Erin Zühlke

http://upload.wikimedia.org/wikipedia/commons/9/9e/Graphen.jpg

Graphene

- perfect two-dimensional crystal
- single layer of carbon atoms
- hexagonal lattice
- unique properties



http://www.jameshedberg.com/img/samples/graphene-simple.jpg

Graphene

Andre Geim

Konstantin Novoselov

http://www.nobelprize.org/nobel_prizes/physics/laureates/2010/

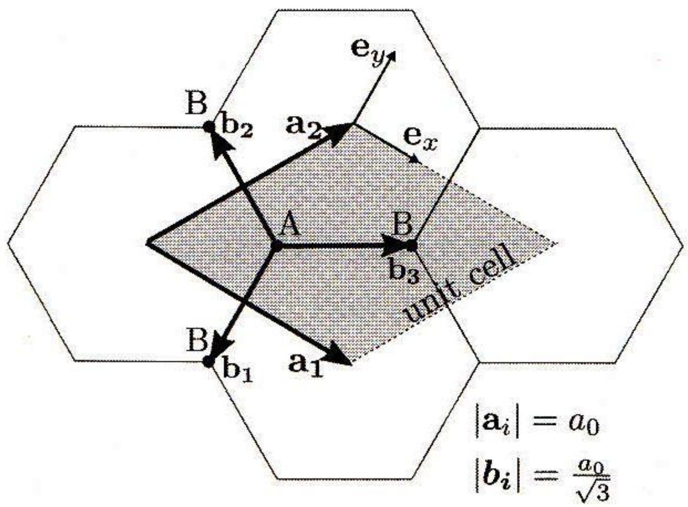
Properties

- surface mass $7.57 \cdot 10^{-7}$ kg $\cdot$ m^{-2}
- tensile strength $1.25 \cdot 10^{11}$ Pa
- thermal conductivity 5000 W / (m $\cdot$ K)
- electrical resistivity 31 $\Omega \cdot$ m

http://de.wikipedia.org/wiki/Graphen

Structure

direct lattice



- $a_1 = a_0(1,0)$
- $a_2 = \frac{a_0}{2}(1, \sqrt{3})$
- $|a_i| = a_0 = 0.246\ nm$

- $b_1 = \frac{a_0}{\sqrt{3}}(0, -1)$
- $b_2 = \frac{a_0}{2}\left(-1, \frac{1}{\sqrt{3}}\right)$
- $b_3 = \frac{a_0}{2}\left(1, \frac{1}{\sqrt{3}}\right)$
- $|b_i| = \frac{a_0}{\sqrt{3}} = 0.142\ nm$

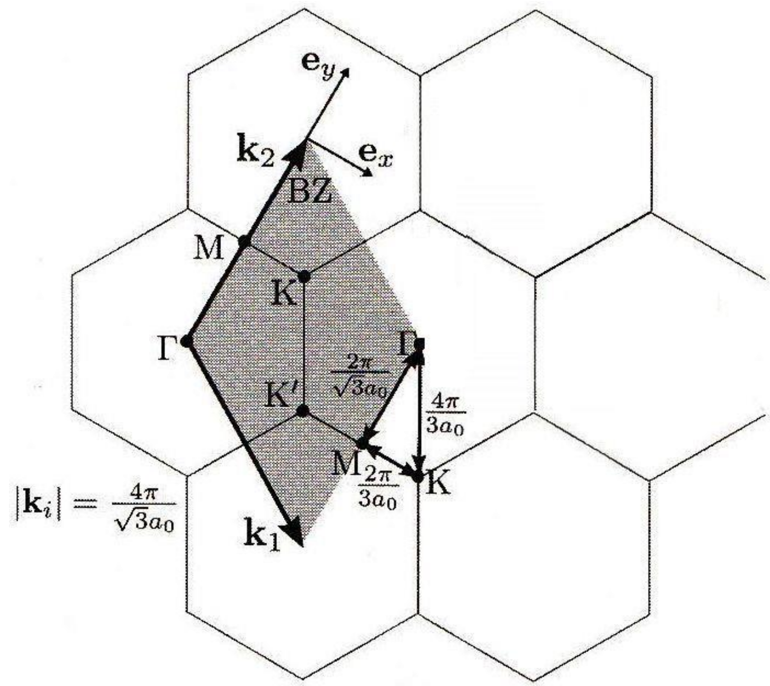
Ermin Malic, Andreas Knorr: Graphene and Carbon Nanotubes 2013

Structure

- $k_1 = \frac{2\pi}{\sqrt{3}a_0}(\sqrt{3}, -1)$
- $k_2 = \frac{4\pi}{\sqrt{3}a_0}(0,1)$

- $\Gamma = 0$
- $K = \frac{1}{3}(k_1 - k_2)$
- $K' = \frac{1}{3}(2k_1 + k_2)$
- $M = \frac{1}{2}k_2$

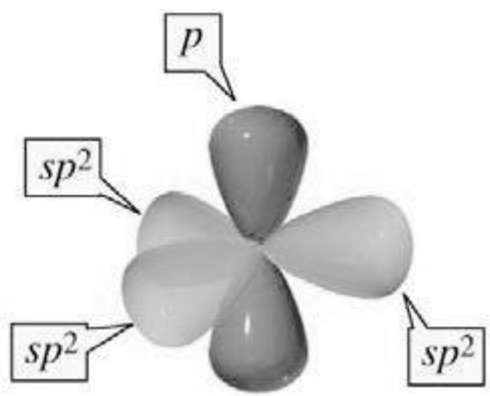
reciprocal lattice



Ermin Malic, Andreas Knorr: Graphene and Carbon Nanotubes 2013

Structure

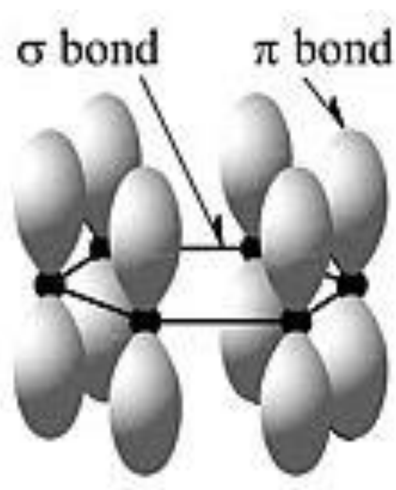
- carbon: $1s^2\ 2s^2\ 2p^2$
- four valence electrons
- 2s and 2p hybridize to form sp^2 orbitals



http://introorganicchemistry.com/basic.html

Structure

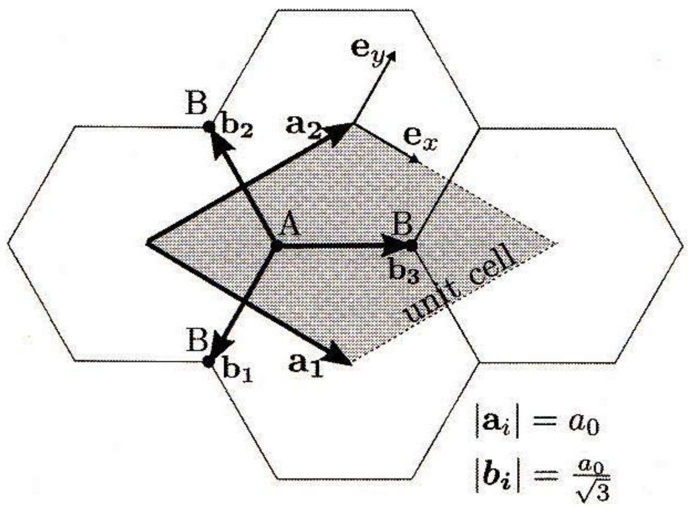
- three $2sp^2$ electrons -> σ-bond
- one 2p electron -> π-bond



http://www.andrew.cmu.edu/user/feenstra/graphene/

Structure

direct lattice



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Tight-Binding

$$e(\vec{k}) = \sum_{j=1}^{3} \exp(i\vec{k} \cdot \overrightarrow{b_j})$$

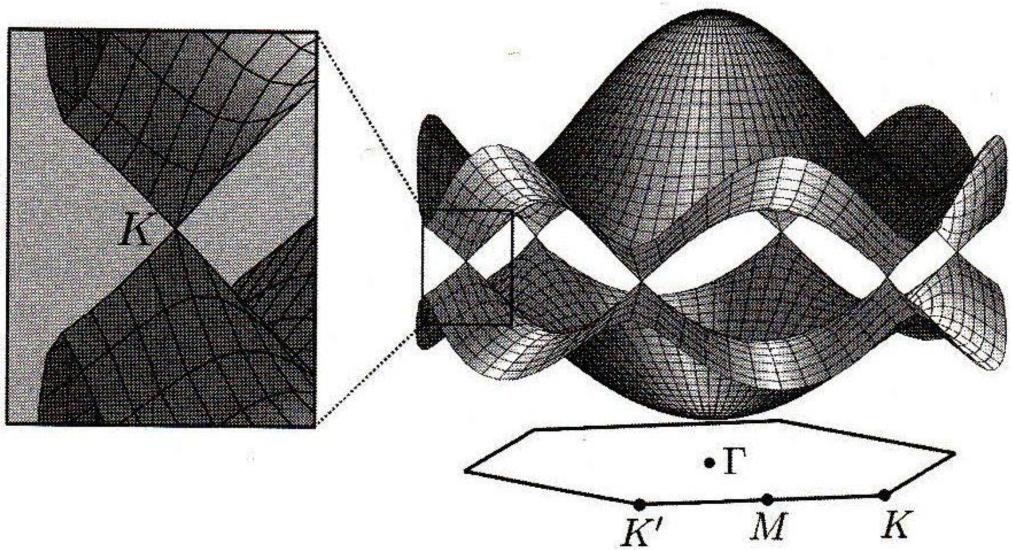
$$\vec{b}_1 = \frac{1}{3}(\vec{a}_1 - 2\vec{a}_2)$$
$$\vec{b}_2 = \frac{1}{3}(-2\vec{a}_1 + \vec{a}_2)$$
$$\vec{b}_3 = \frac{1}{3}(\vec{a}_1 + \vec{a}_2)$$

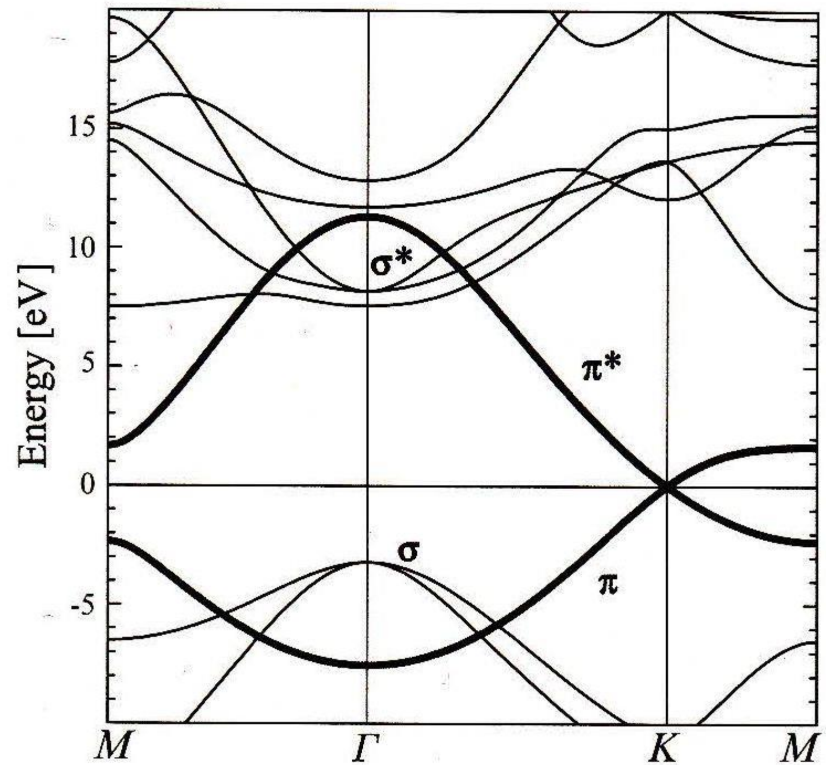
$$|e(\vec{k})| = [3 + 2\cos\left(\vec{k} \cdot (\vec{a}_1 - \vec{a}_2)\right) + 2\cos(\vec{k} \cdot \vec{a}_2) + 2\cos(\vec{k} \cdot \vec{a}_1)]^{\frac{1}{2}}$$
$$= [3 + 2\cos(a_0 k_y) + 4\cos\left(\frac{\sqrt{3}a_0}{2}k_x\right)\cos(\frac{a_0}{2}k_y)]^{\frac{1}{2}}$$

$$\varepsilon_k{}^{\pm} = \pm\gamma_0|e(\vec{k})|$$

γ_0 tight-binding parameter

Band Structure





band structure of graphene
conduction and valence band along
the first Brillouin zone

band structure along the
high-symmetry direction
K-Γ-M-K'

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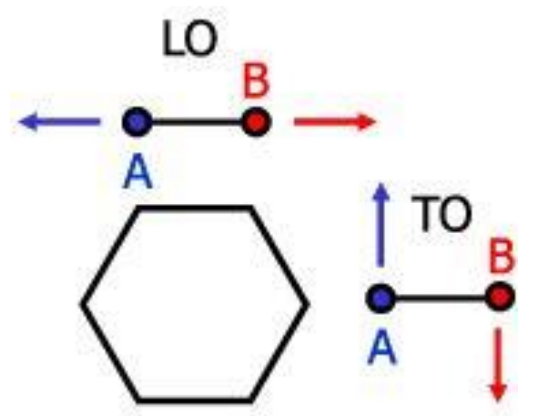
Vibrational Properties

Newtonian coupled equation: $\vec{u}_n \omega^2 = -\sum_m \Phi_{m,n} \vec{u}_n$

dynamical matrix: $\Phi_{m,n}$

$$\vec{u}_n^{A,B} \sim e^{i\,\vec{k}\,\cdot\,\vec{R}_n^{A,B}}$$

equilibrium position: $\vec{R}_n^{A,B}$

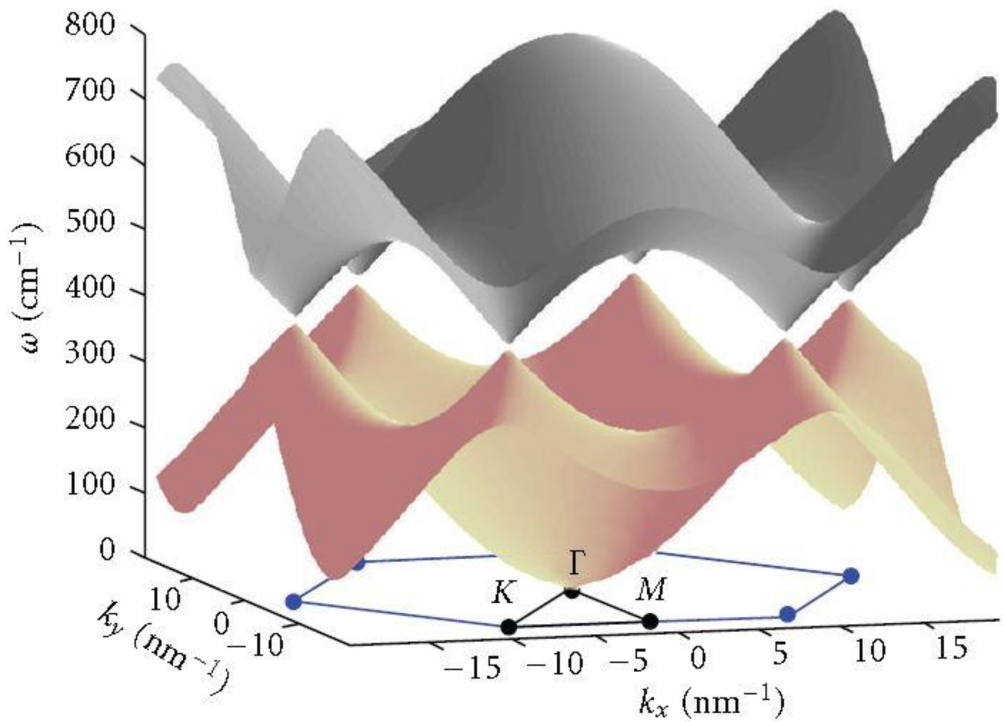


optical in-plane vibrations

http://iopscience.iop.org/0953-8984/25/14/144201/article

Cooper, Daniel R., et al. "Experimental review of graphene." ISRN Condensed Matter Physics 2012 (2012).

Vibrational Properties



out-of-plane phonon mods
gray: ZO (optical) and pink ZA (acoustic)

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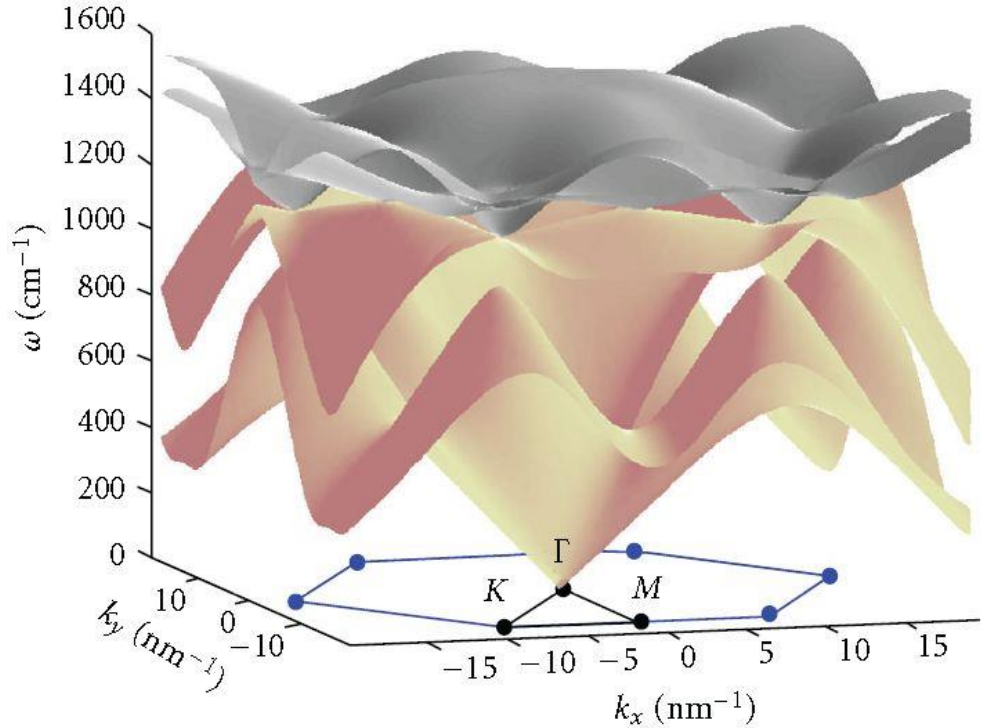
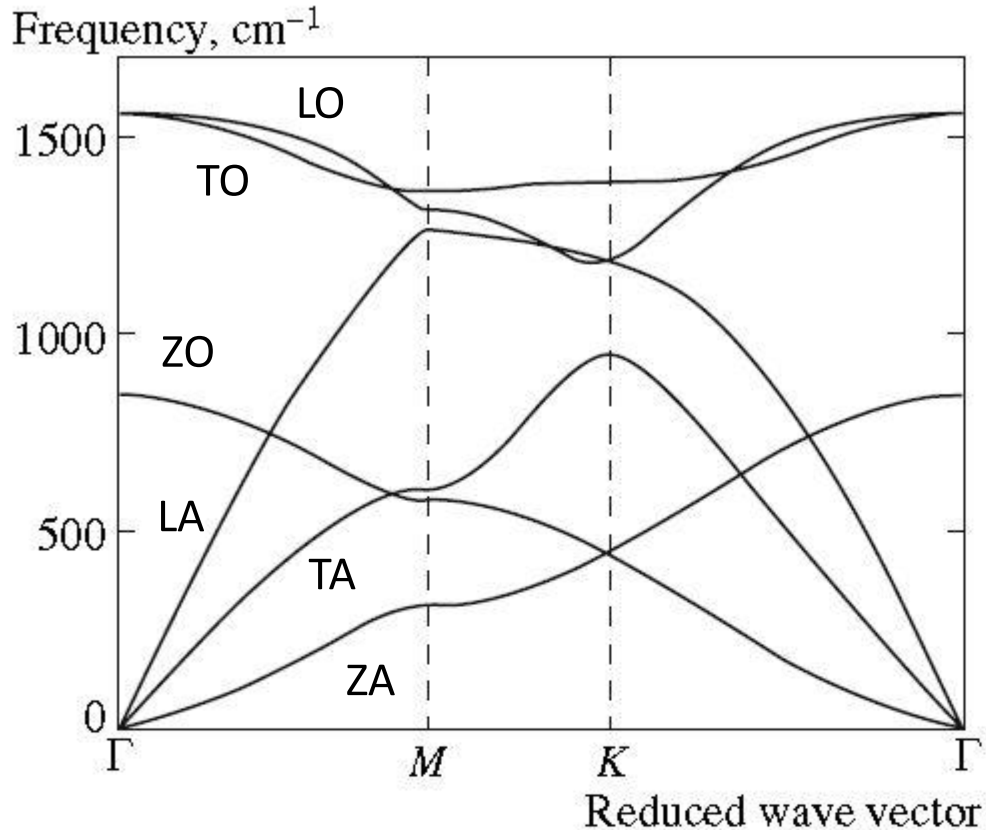
Vibrational Properties



in-plane phonon mods
gray: LO, TO and pink: LA, TA

Cooper, Daniel R., et al. "Experimental review of graphene." ISRN Condensed Matter Physics 2012 (2012).

Vibrational Properties



all modes along the special symmetry points

Cooper, Daniel R., et al. "Experimental review of graphene." ISRN Condensed Matter Physics 2012 (2012).