Lenosky's energy and the phonon dispersion of graphene

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Lenosky Model

•Introduced for negatively curved graphene
•Takes into account orbital overlap due to curvature

$$U L_d = \frac{\epsilon_0}{2} \sum_{<ij>} \left(|\mathbf{r}_{ij}| - |\mathbf{e}_{ij}|\right)^2$$

Stretching

$$U L_a = \epsilon_1 \sum_i \left(\sum_{<j>} \hat{\mathbf{r}}_{ij} \right)^2$$

~ Dangling bond

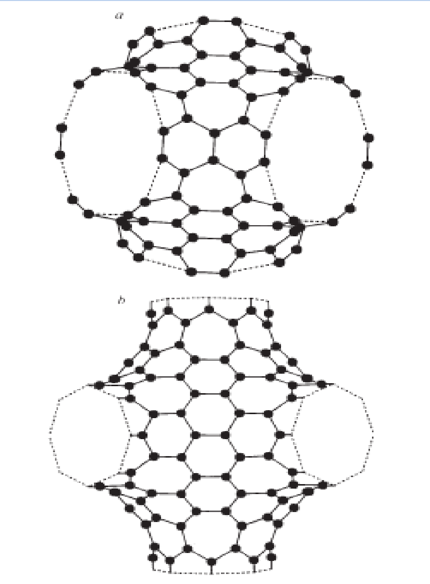
$$U L_{b1} = \epsilon_2 \sum_{<ij>} \left(1 - \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j\right)$$

π-π overlap

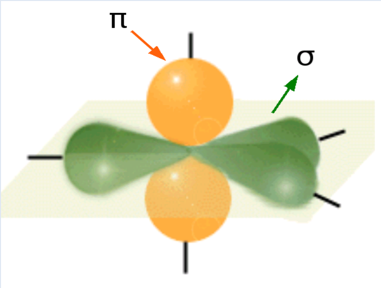
$$U L_{b2} = \epsilon_3 \sum_{<ij>} \left(\hat{\mathbf{n}}_i \cdot \hat{\mathbf{r}}_{ij}\right)\left(\hat{\mathbf{n}}_j \cdot \hat{\mathbf{r}}_{ji}\right)$$

π-σ overlap

Schwarzite



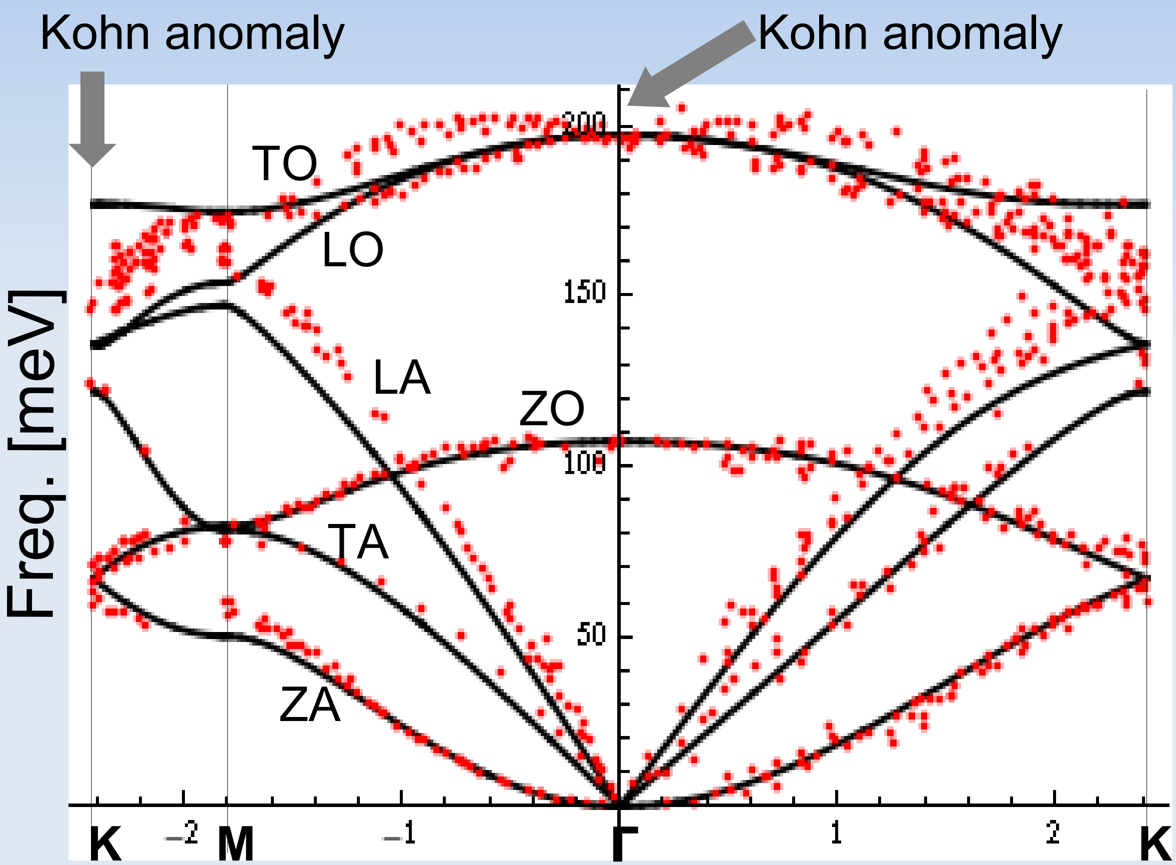
Lenosky *et al.*
Nature **355** 333 (1992)



We calculate the phonon dispersion for the Lenosky model

Hybrid model

We add the bond-bending term to Lenosky's energy:



Good Fit!

Five free parameters:

ε_0=30 eV → stretch

ε_1=1.34 eV → dangling

ε_2=0.23 eV → π-π

ε_3=1.16 eV → π-σ

β=2.40 eV → bending

π-σ → overlap responsible for ZO flattening

→ dominates over π-π overlap