KINKS IN COULOMB’S CHAINS

- Kinks in Coulomb’s chains

Juan FR Archilla
Group of Nonlinear Physics Lineal (GFNL),
Department of Applied Physics I
University of Sevilla, Spain
http://grupo.us.es/gfnl
With Yury Kosevich
Semenov Institute of Chemical Physics
Russian Academy of Sciences, Moscow, Russia
And Mike Russell
Heriot-Watt University

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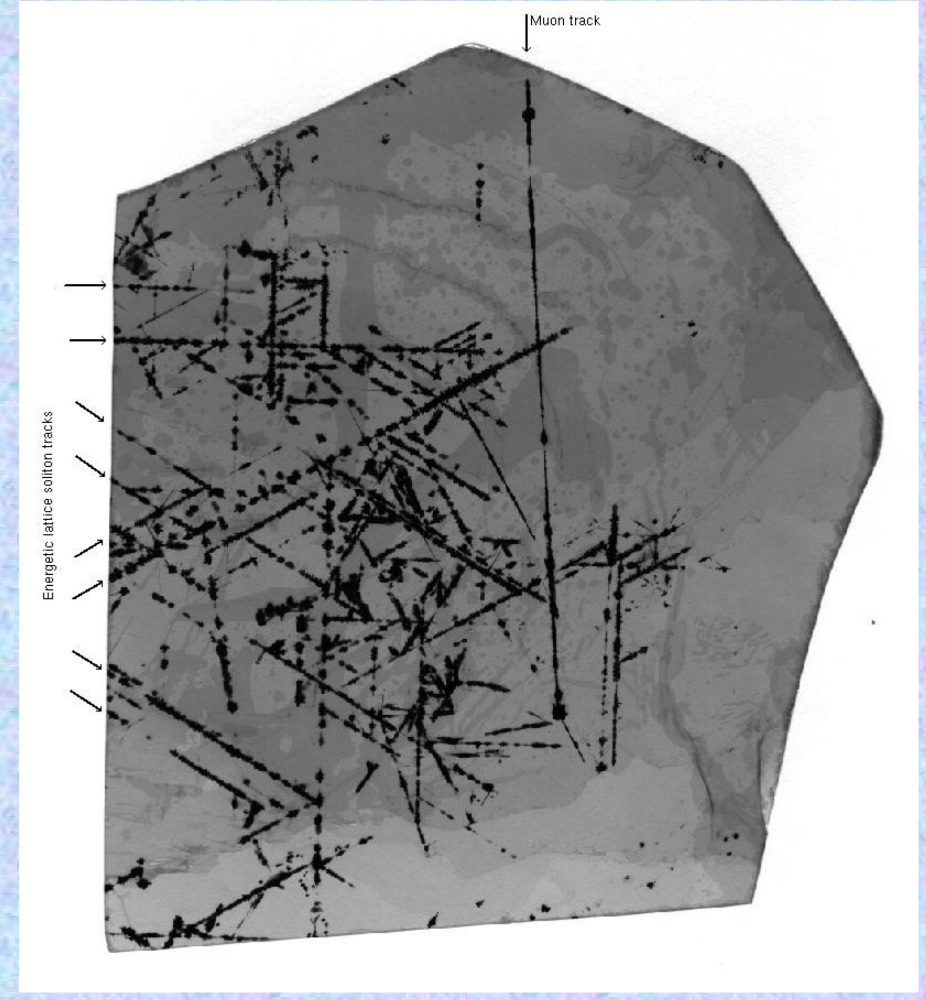
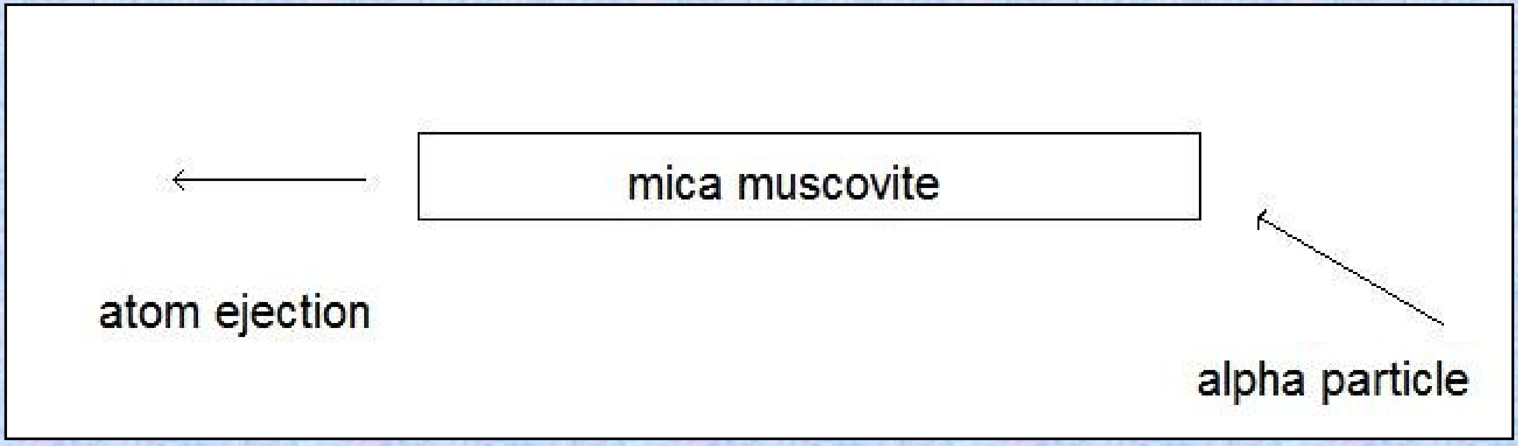
Record of moving excitations in mica muscovite: quodons (Russell)



- 99.9% of the tracks are supposed to be lattice localized exitations or quodons?
- They travel along lattice directions
- They travel long distances (mm)
- They have enough energy to eject an atom

Schlößer, D., Kroneberger, K., Schosnig, M., **Russell, F.M**. & Groeneveld, K.O. (1994). Search for solitons in solids. *Radiation Measurements* 23, 209-213.

Experimental evidence of travelling excitations in mica muscovite

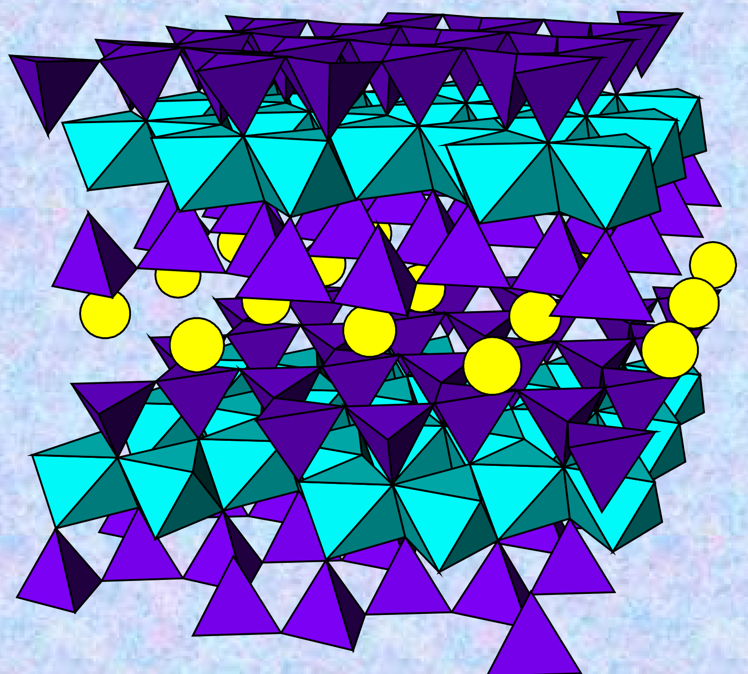


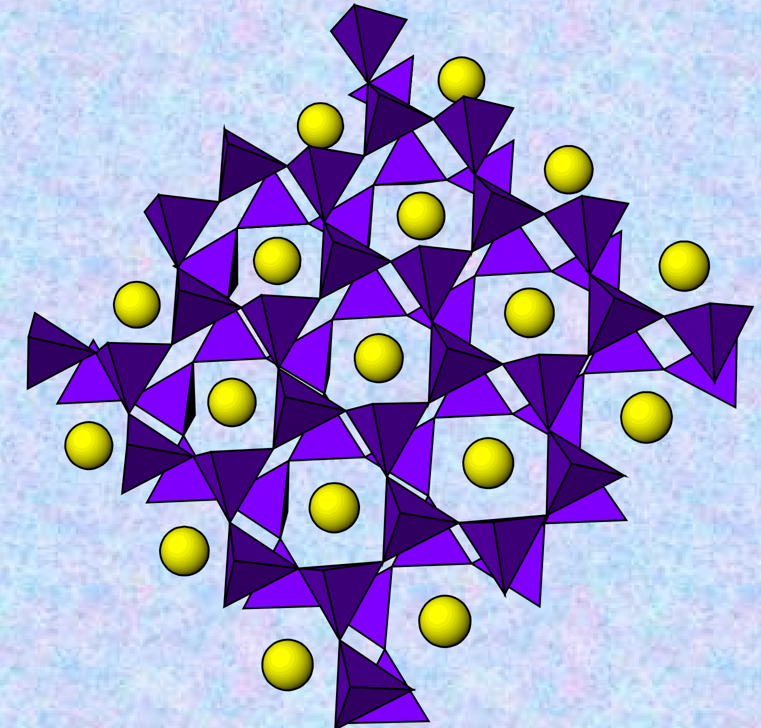
Trajectories along lattice directions within the K^+ layer

Russell, F.M., Eilbeck, J.C. (2007). Evidence for moving breathers in a layered crystal insulator at 300K. *Europhysics Letters* 78, 1004, 1-5.

Mica muscovite. Cation layers

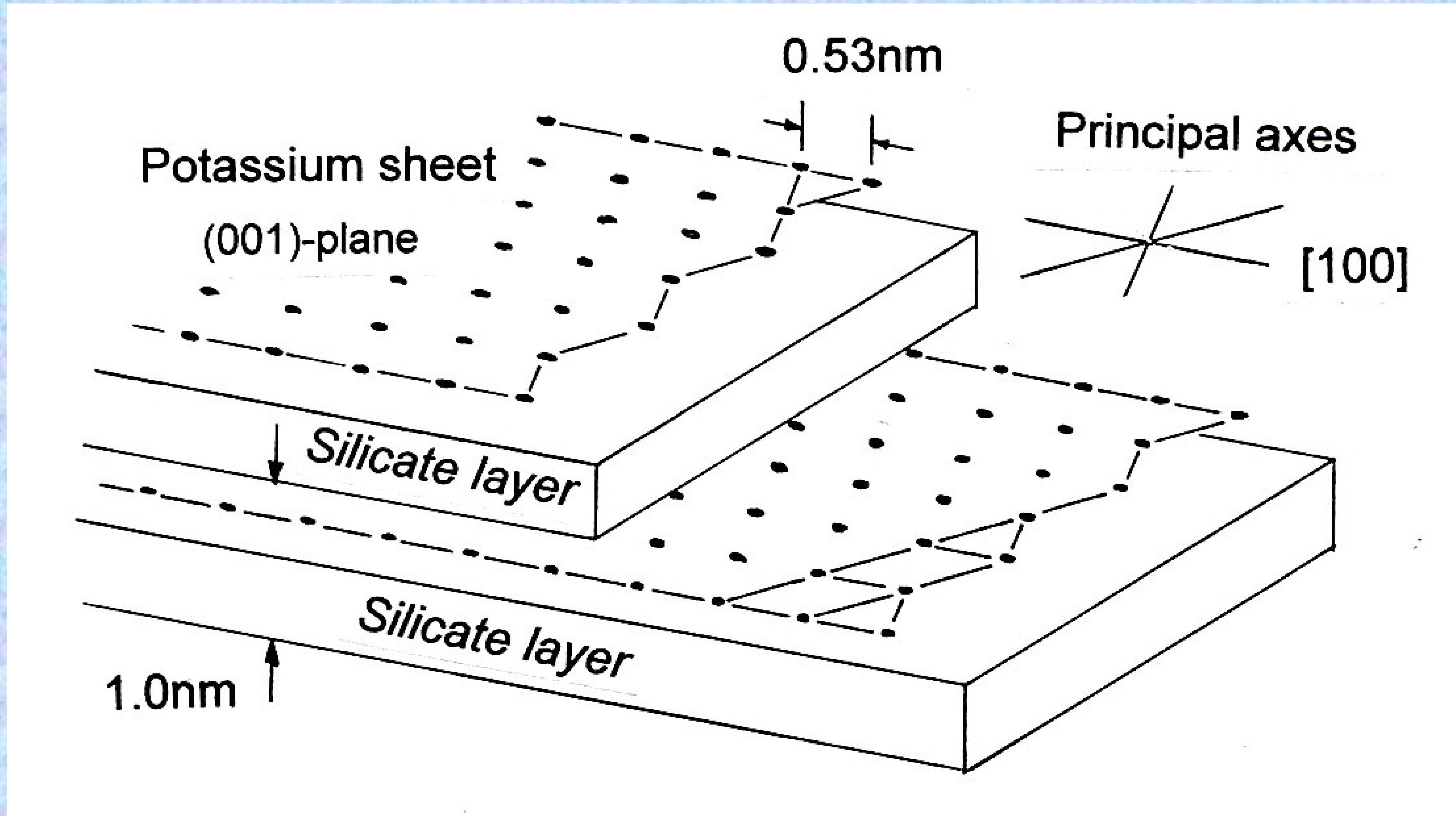
$K_2[Si_6Al_2]^{IV}[Al_4]^{VI}O_{20}(OH)_4$





K+

Mica muscovite. Cation layers

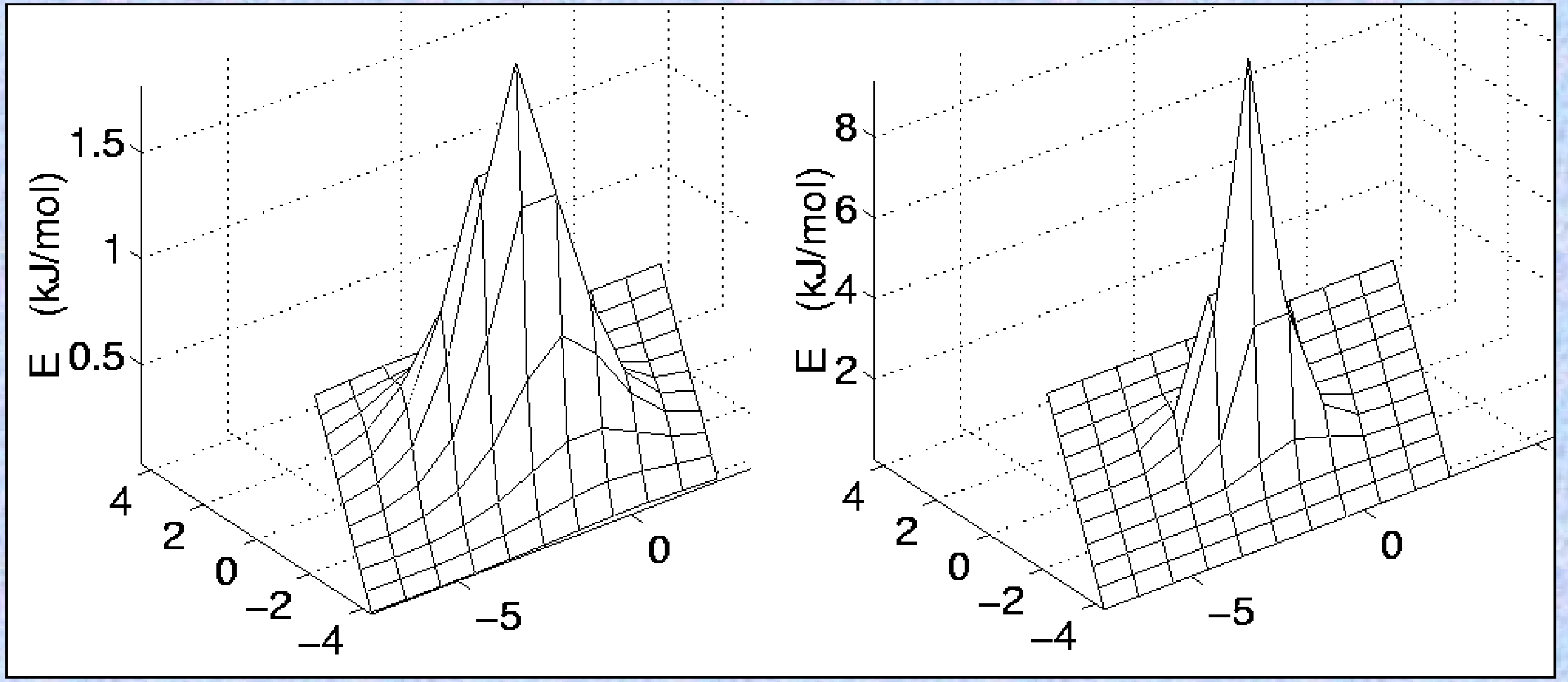


Courtesy of Mike Russell

Transversal breathers have low energies and move slowly

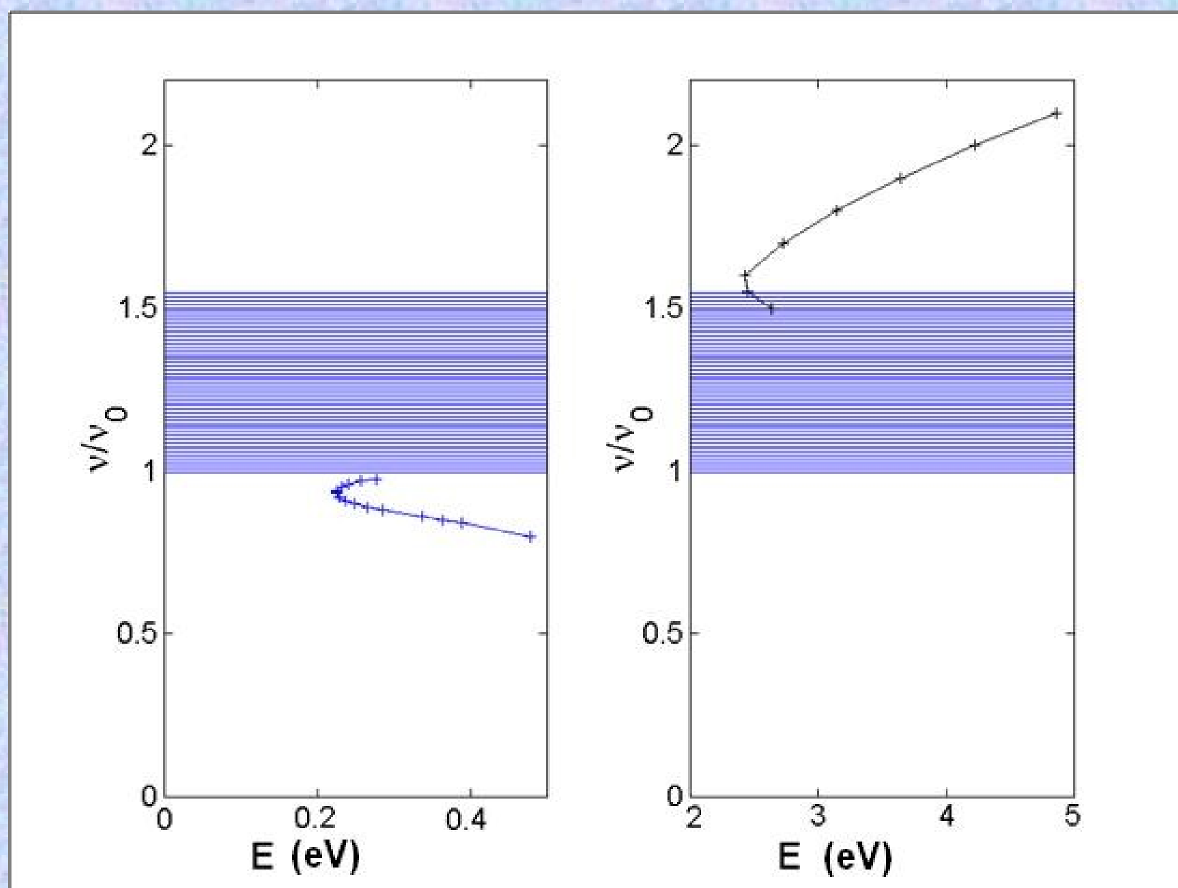
Soft breather, E=0.2~0.4 eV ν~ 5·10^{12} Hz

Hard breather. E ~0.36eV



Dubinko, V.I., Selyshchev, P.A. & Archilla, J.F.R. (2011). Reaction-rate theory with account of the crystal anharmonicity. *Phys. Rev.* E 83, 041124, 1-13

Transversal soft and hard breather spectra

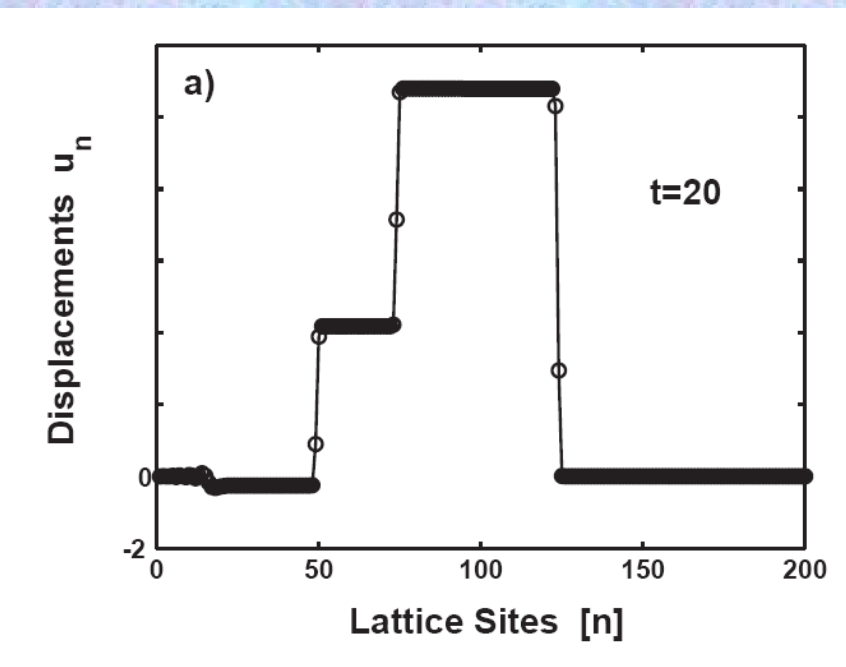


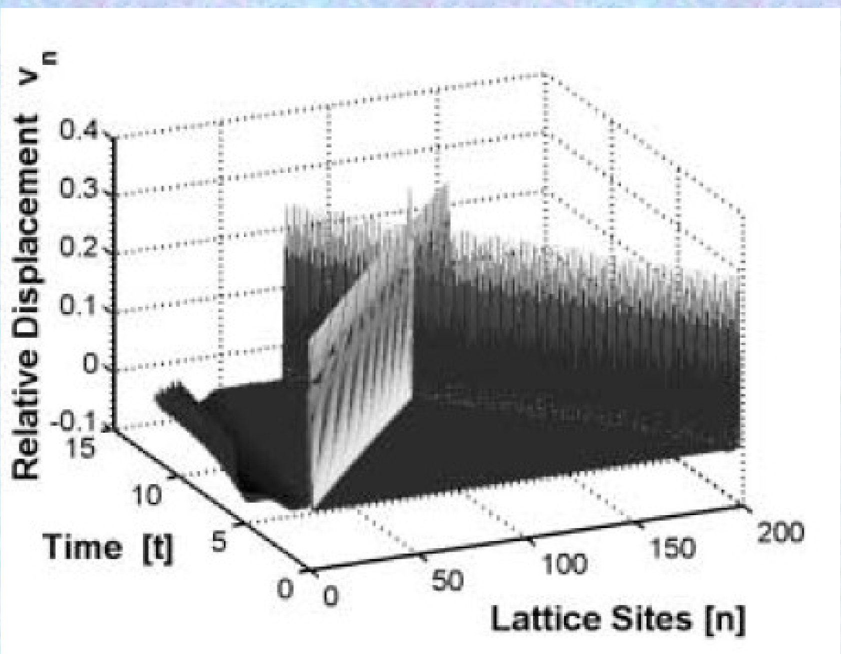
ν_0= 167.5cm^{-1}

~ 5·10^{12} Hz

~20 meV

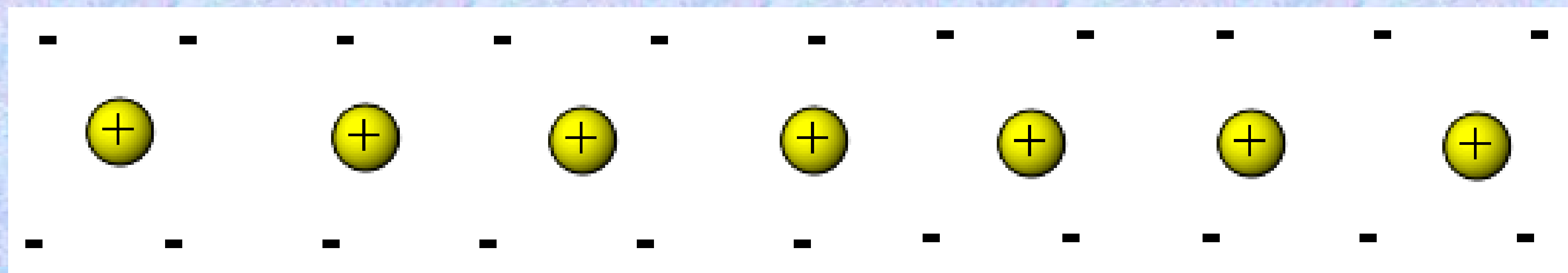
Supersonic kinks move very fast and have large energies, but they are too much transversal.





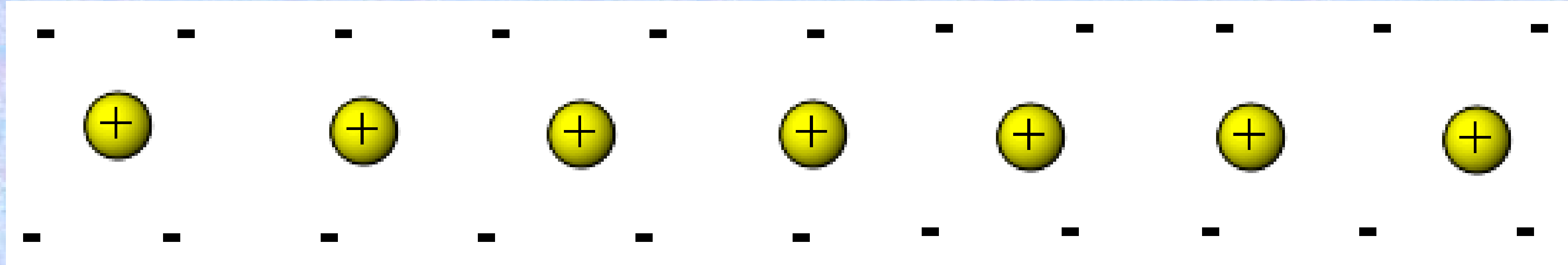
Yu A Kosevich, Yu. A., Khomeriki, R & Ruffo, S. (2004). Supersonic discrete kink-solitons and sinusoidal patterns with “magic” wave number in anharmonic lattices. *Europhys. Lett.*, 66, 21–27.

Coulomb's chains



- Longitudinal perturbations
- Cations are in a negative medium so:
  - Coulomb's repulsion is rapidly screened
  - The system does not explode
  - We discard long range and more than nearest neighbour interactions.
- Negative charge at the borders keep cations inside
- Obstacle to movement would come from steric effects given by weak Van der Waals forces and electric ones by Pauli repulsion, given by overlapping electron orbitals

Model with fixed ends

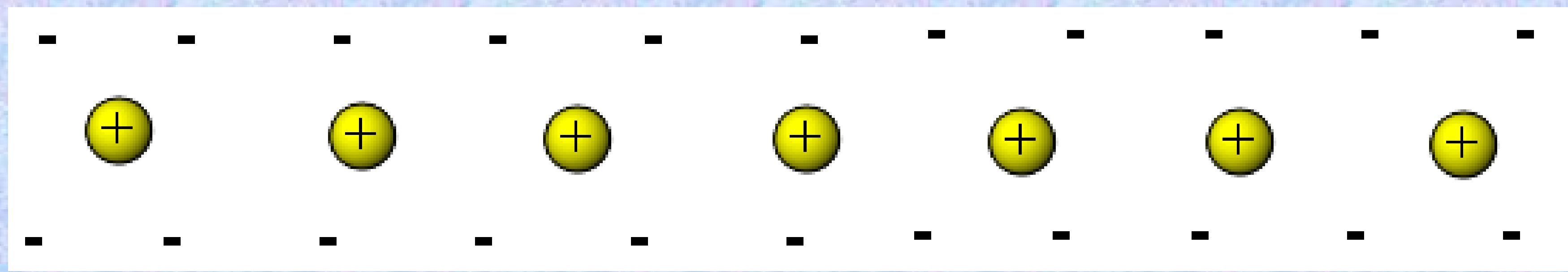


$$m_K \frac{d^2 x_n}{dt^2} = -\frac{Ke^2}{(x_{n+1} - x_n)^2} + \frac{Ke^2}{(x_n - x_{n-1})^2}$$

$$\ddot{u}_n = -\frac{0.5}{(1 + u_{n+1} - u_n)^2} + \frac{0.5}{(1 + u_n - u_{n-1})^2}$$

$$\text{Units:} \quad a = 5.19\,\text{A}, \quad \tau = \frac{1}{\omega_0} = \sqrt{\frac{m_K a^3}{2K_C e^2}} = 0.14\,\text{ns}$$

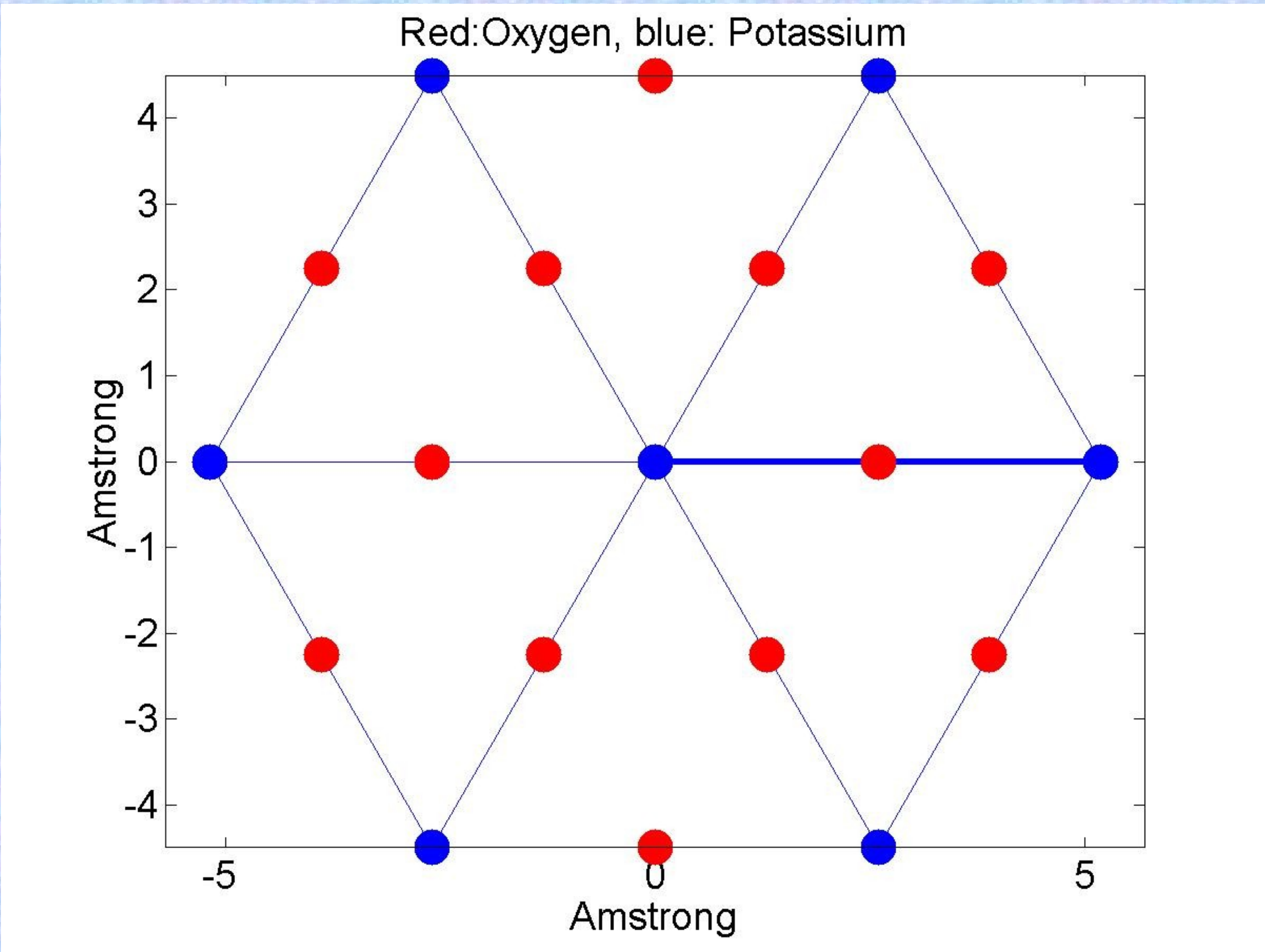
What’s nice about repulsión?



- Repulsión is a good stabilizer
- Forces decay rapidly, fewer phonons.
- We now that it is there
- Forces that increase with the distance are not physical as the linerarized system:

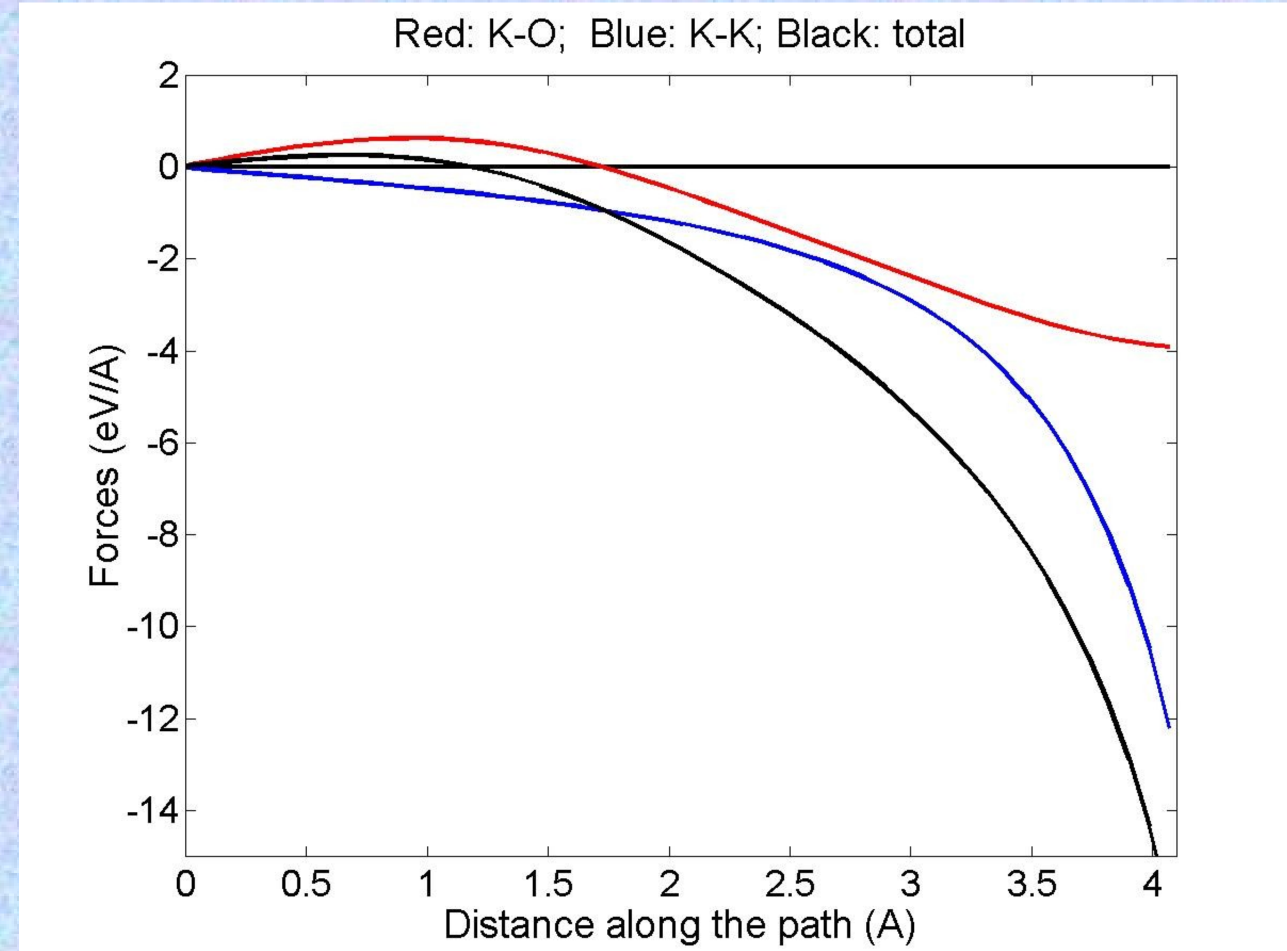
$$\ddot{u}_n = (u_{n+1} - u_n) - (u_n - u_{n-1})$$

Is the model absurd?



Muscovite empirical potentials

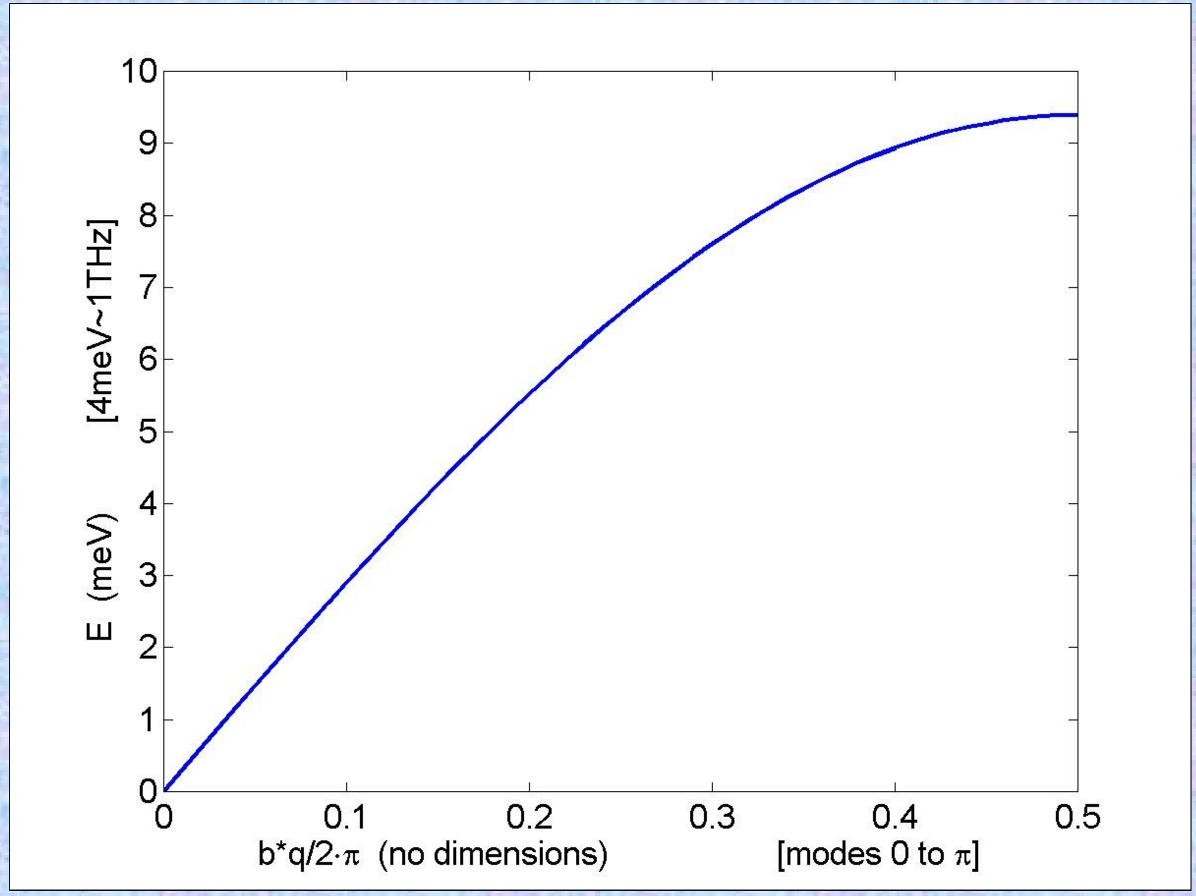
Short range K-O: $U = 65269.7 \exp(-\frac{r}{0.213\text{A}})\text{eV}$



Coulomb interaction

$K^+ - O^{-2}$ and $K^+ - K^+$

Phonon spectra (1)



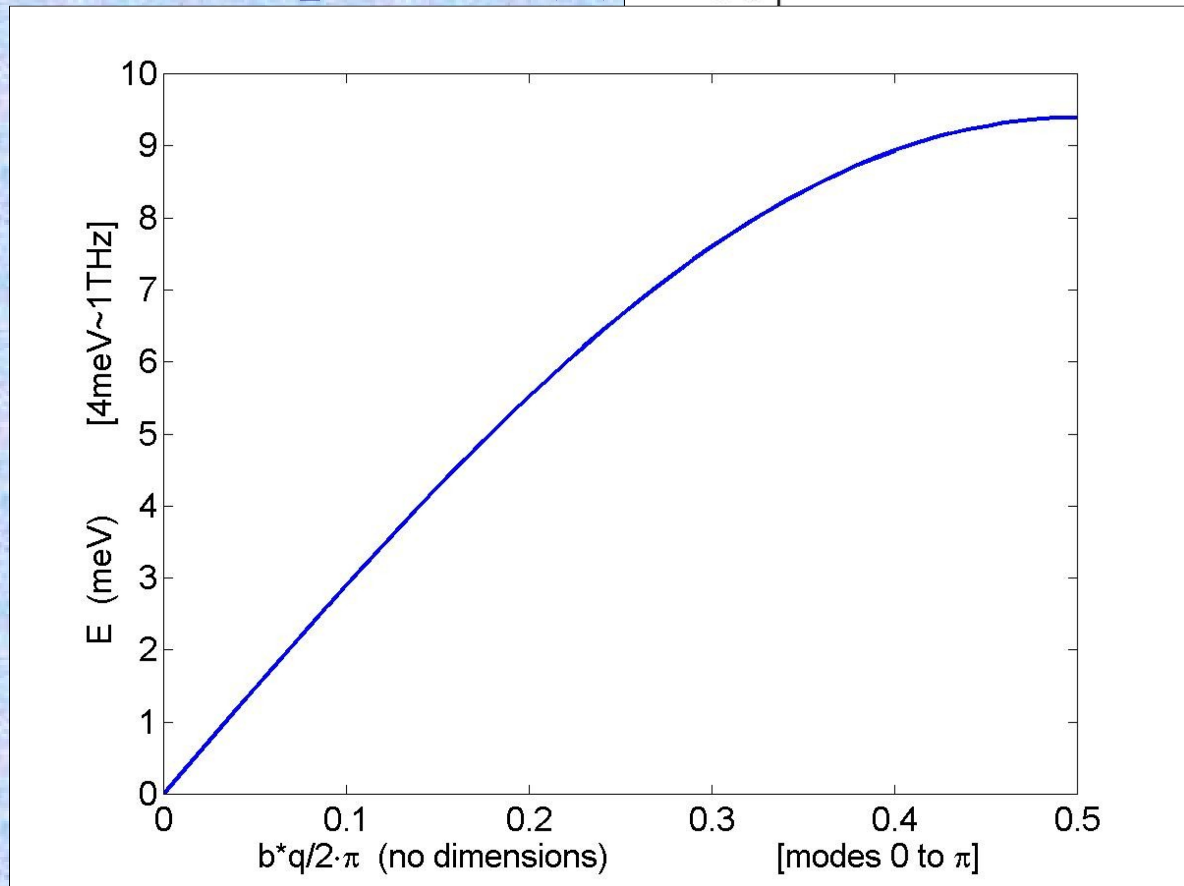
$$E = 2\hbar\omega_0 \sin(\frac{q}{2})$$

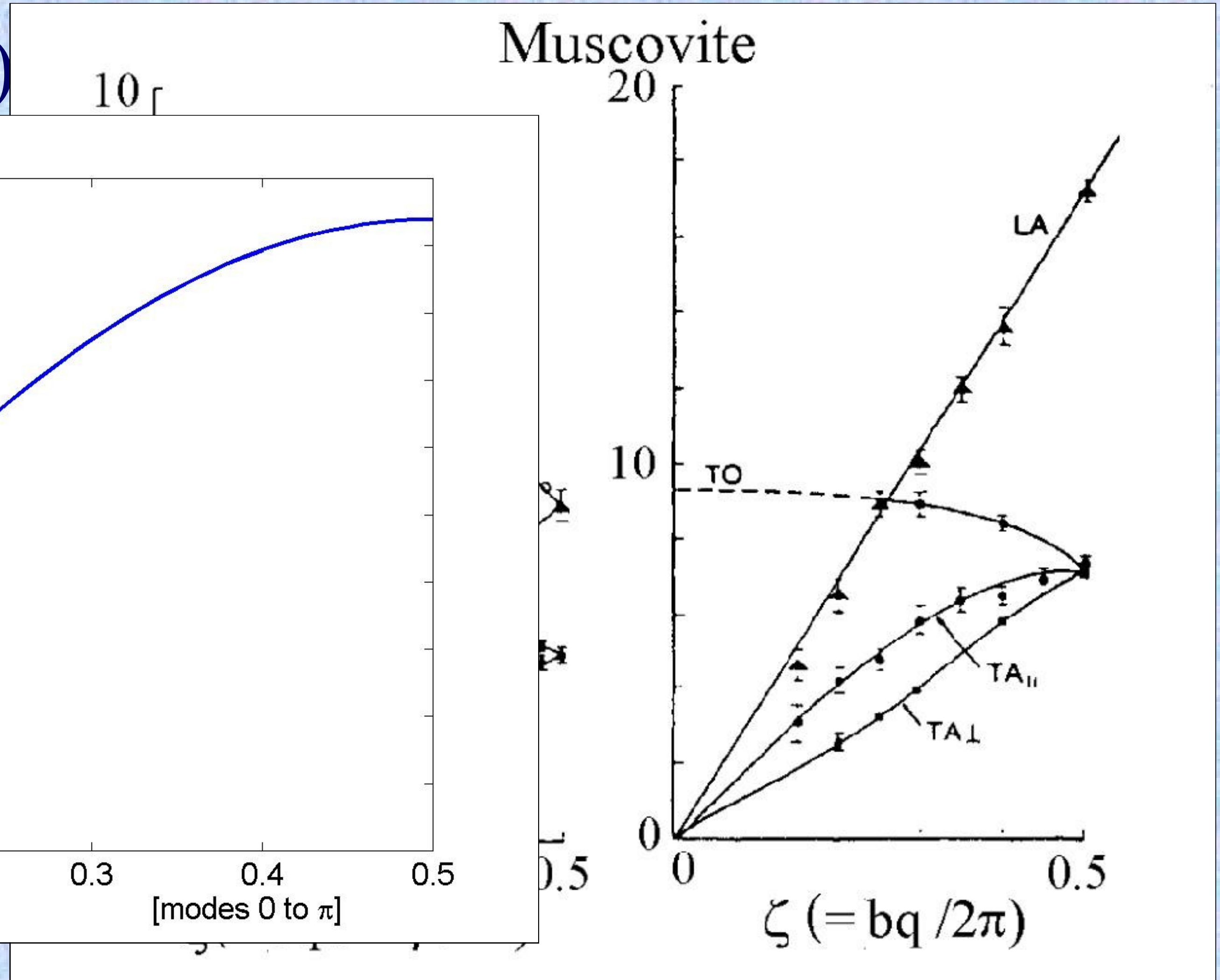
$$\omega_0 = \sqrt{\frac{2K_C e^2}{m_K a^3}}$$

$$f_0 = 1.13\text{THz}$$

SL Chaplot et al. , Inelastic neutron scattering and lattice dynamics of minerals, *Eur. J. Min.* 14, 291 (2002)

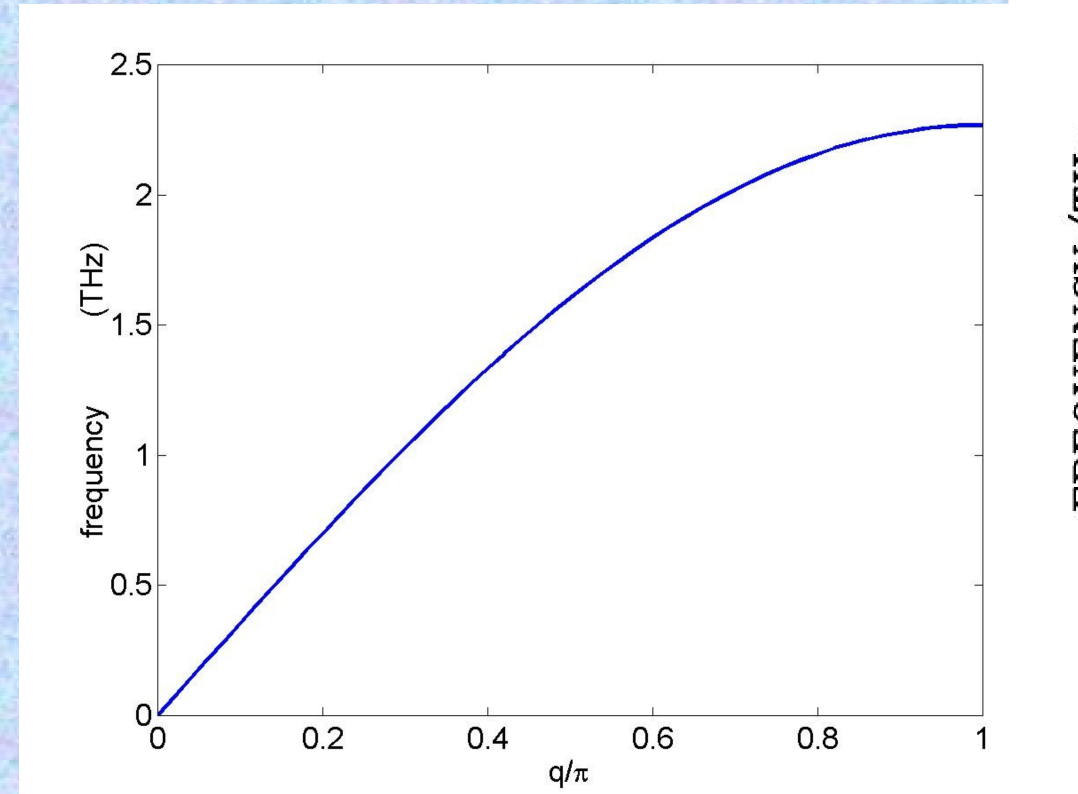
Phonon spectra (2)

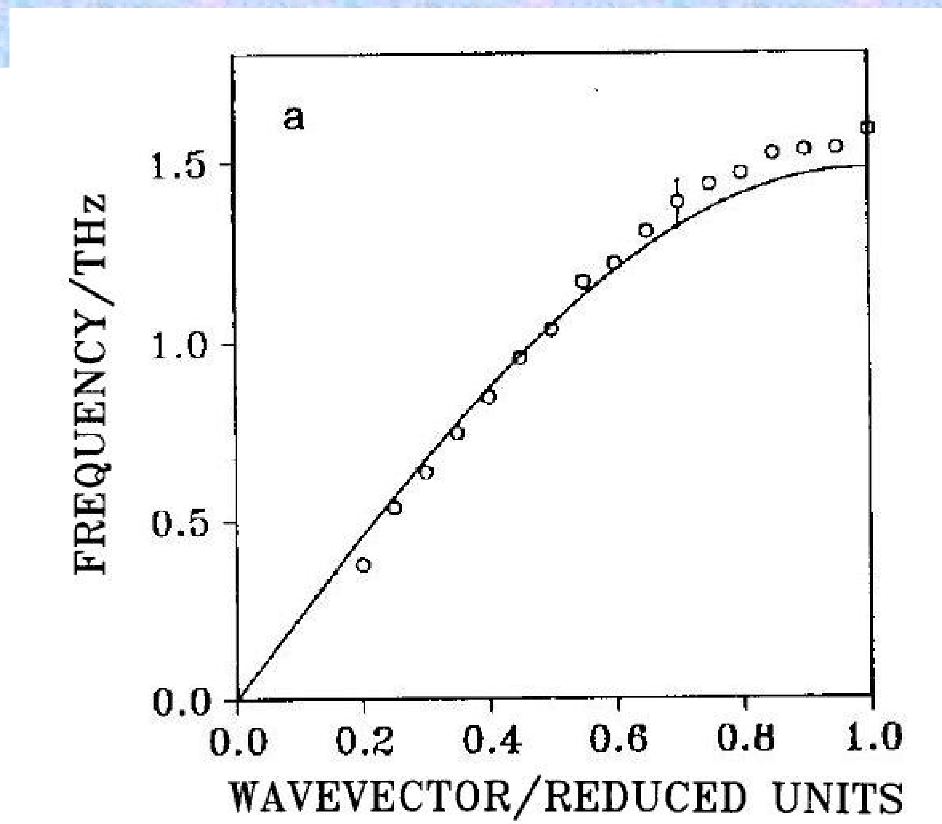




N Wada and WA Kamitakahara, Inelastic neutron and Raman scattering studies of muscovite and vermiculite layered silicates, Phys. Rev. B 43, 2391 (1991)
SL Chaplot et al. , Inelastic neutron scattering and lattice dynamics of minerals, *Eur. J. Min.* 14, 291 (2002) .

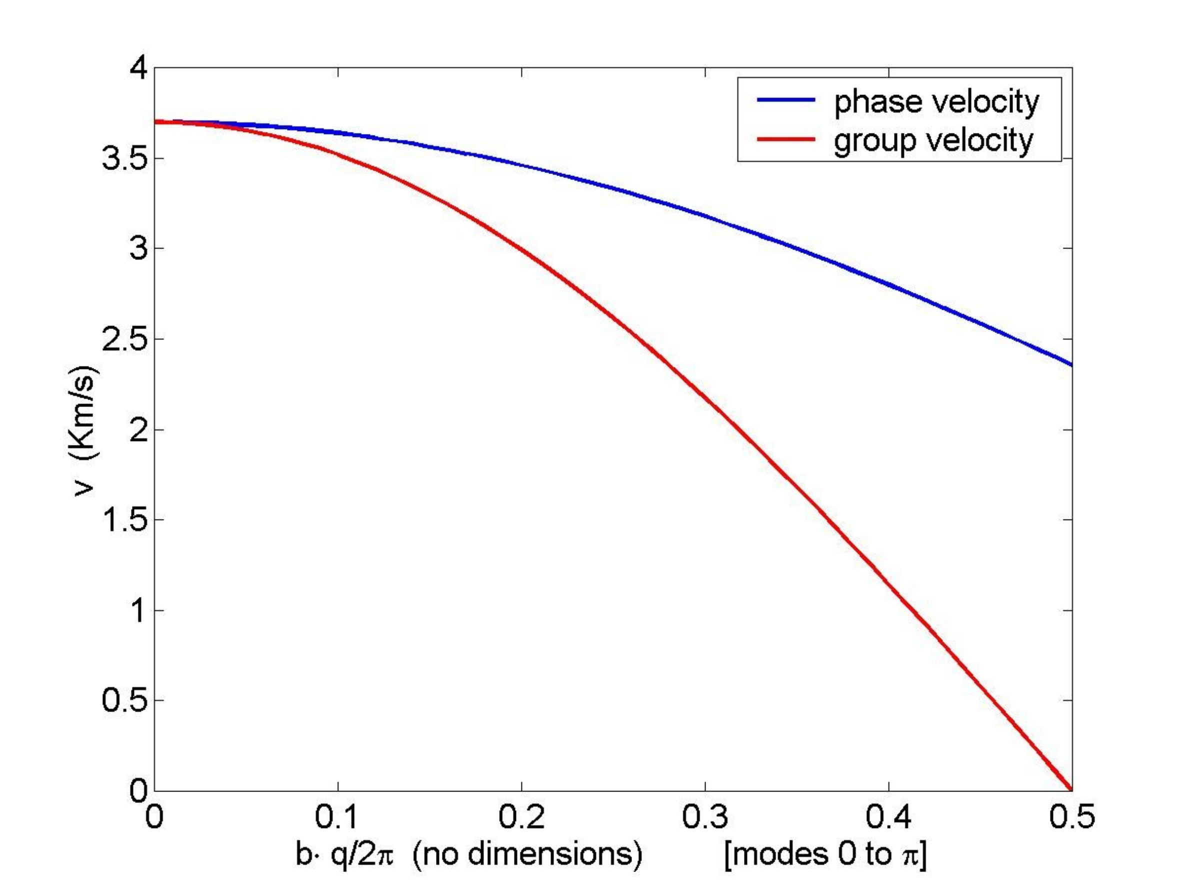
Phonon spectra (3)





D.R. Collins, W.G. Stirling , C.R.A. Catlow and G. Rowbotham Determination of Acoustic Phonon Dispersion Curves in Layer Silicates by Inelastic Neutron Scattering.and Computer Simulation Techniques. *Phys. Chem. Minerals.* 19: 520-527 (1993) .

Sound velocities



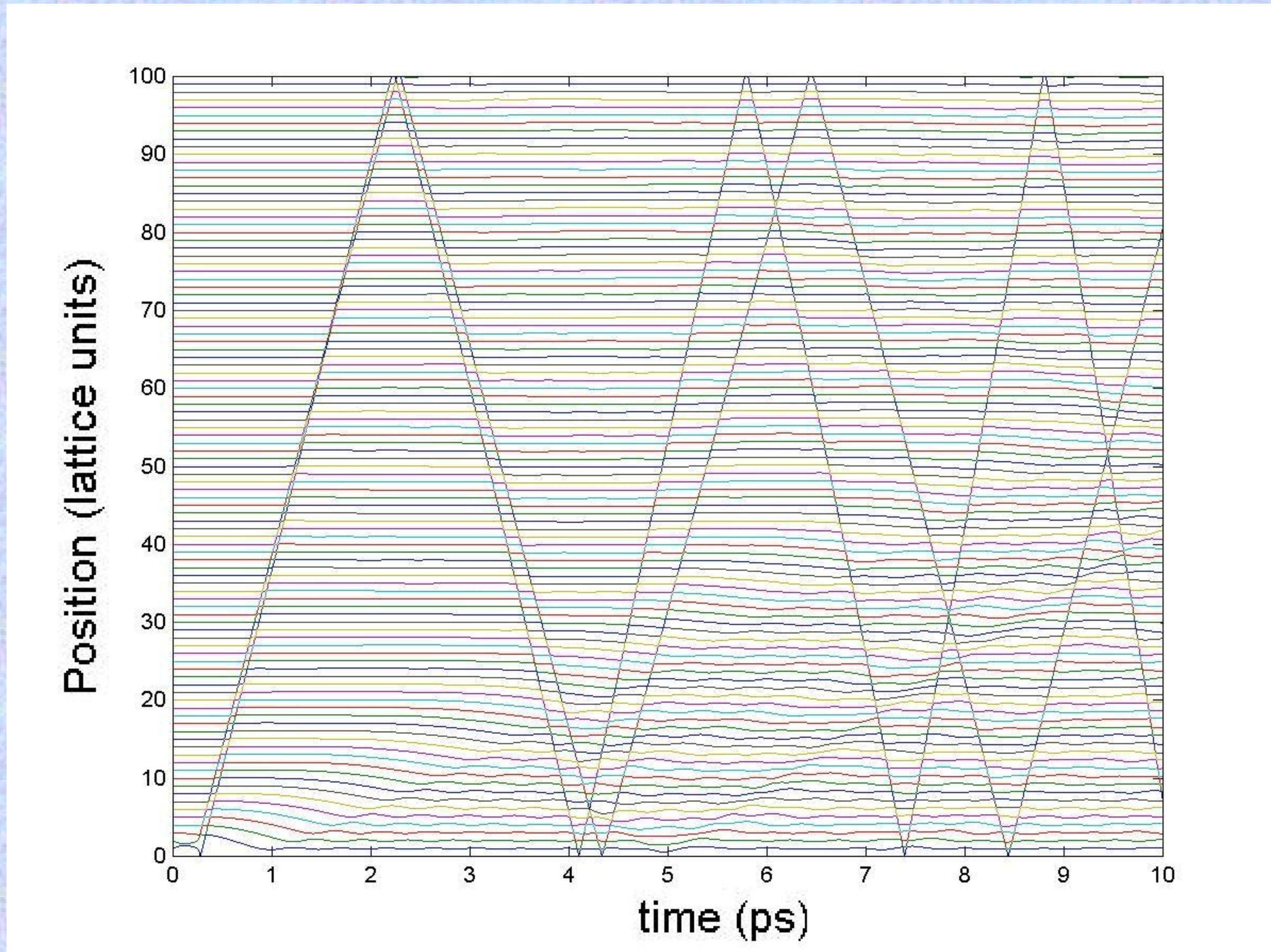
$$v_{ph} = \frac{2\omega_0 a \sin(\frac{q}{2})}{q}$$

$$v_{group} = \omega_0 a \cos(\frac{q}{2})$$

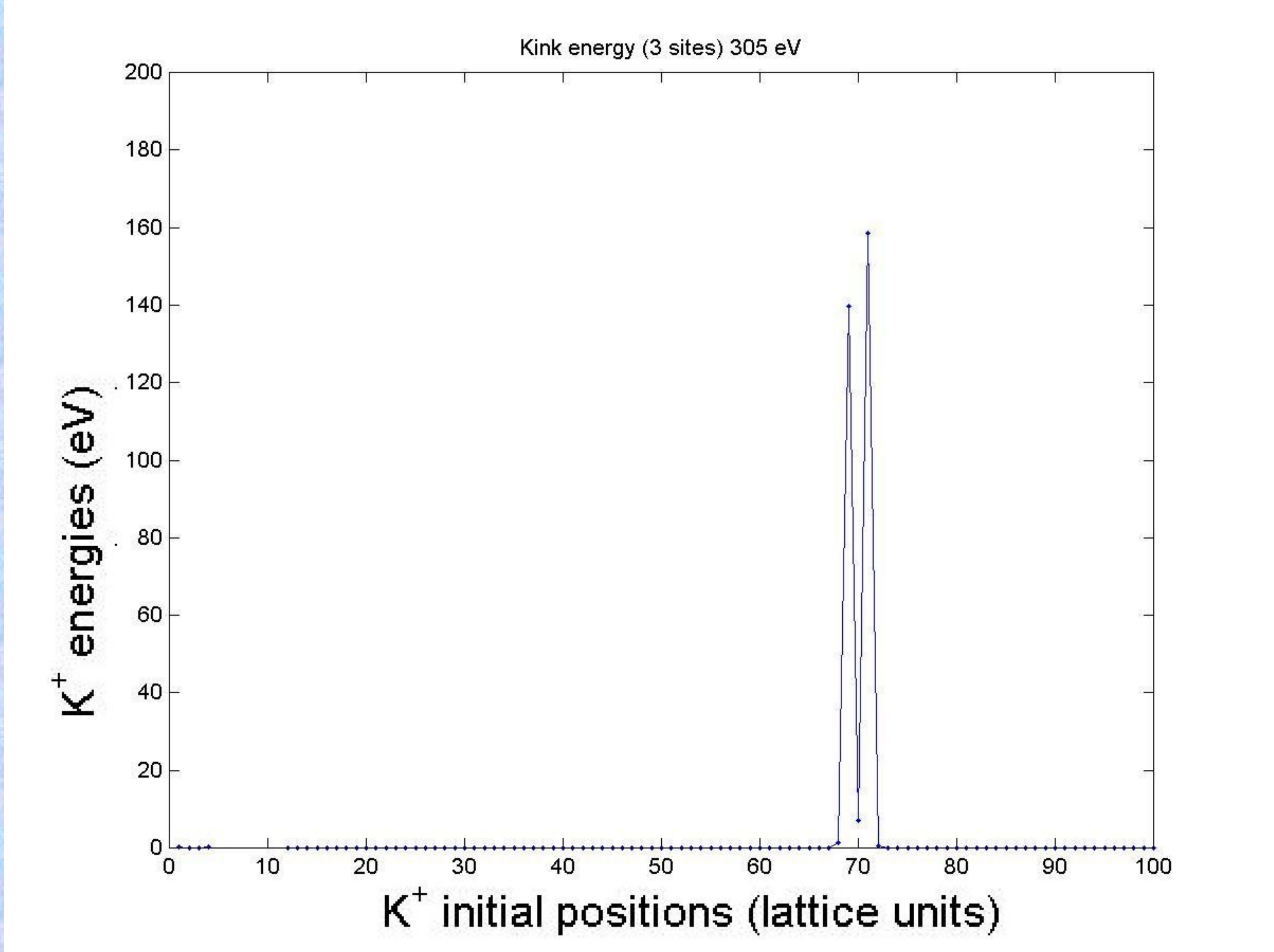
Esperimental
sound velocity: 3.4-3.7 km/s

G. Brudeylins, D. Schmicker, Elastic and inelastic helium atom scattering at a cleaved mica sheet. *Surface Science*, 333: 237-242 (1995).

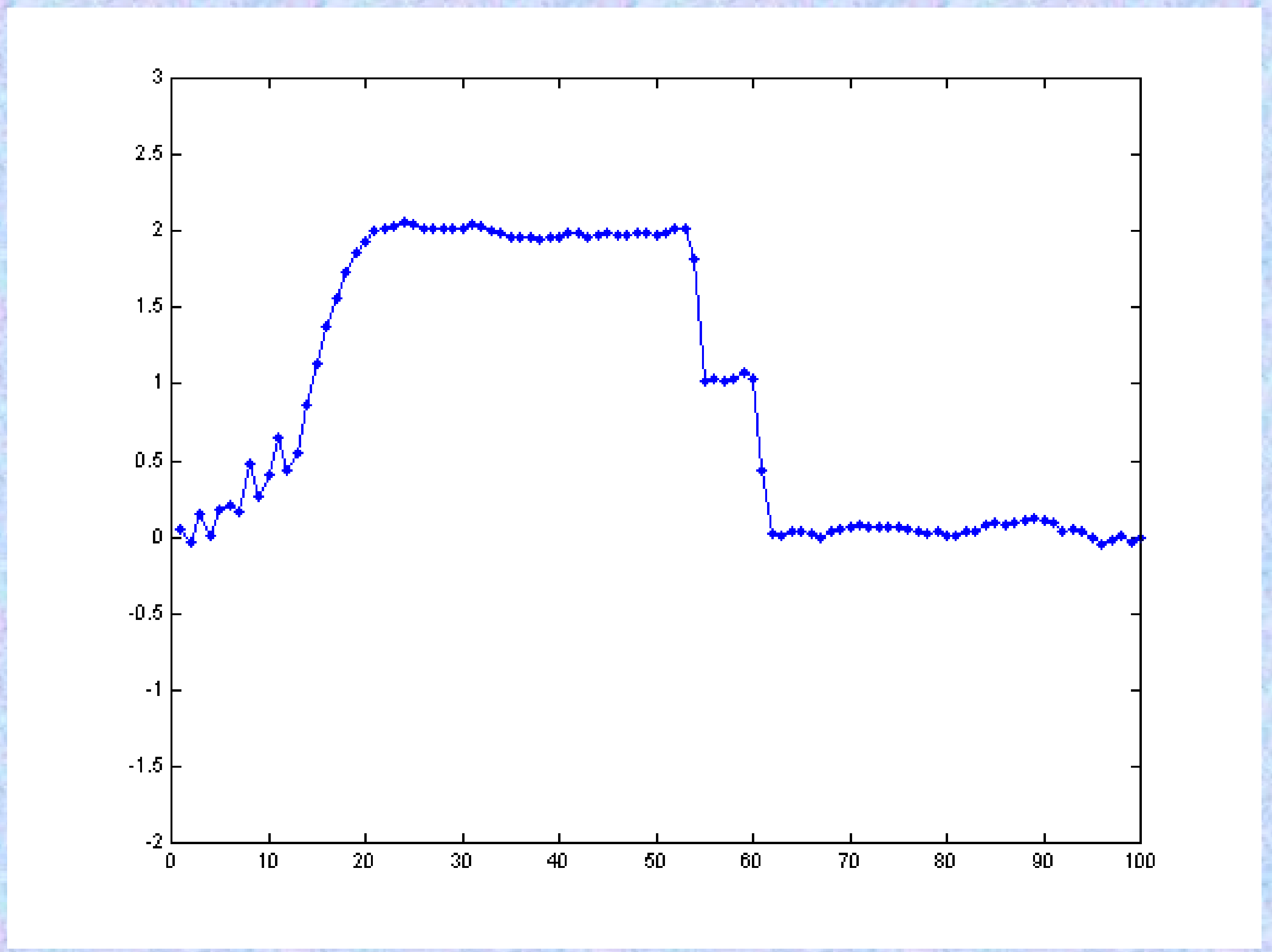
Simulations kink: 26 km/s; phonons: 3.2 km/s



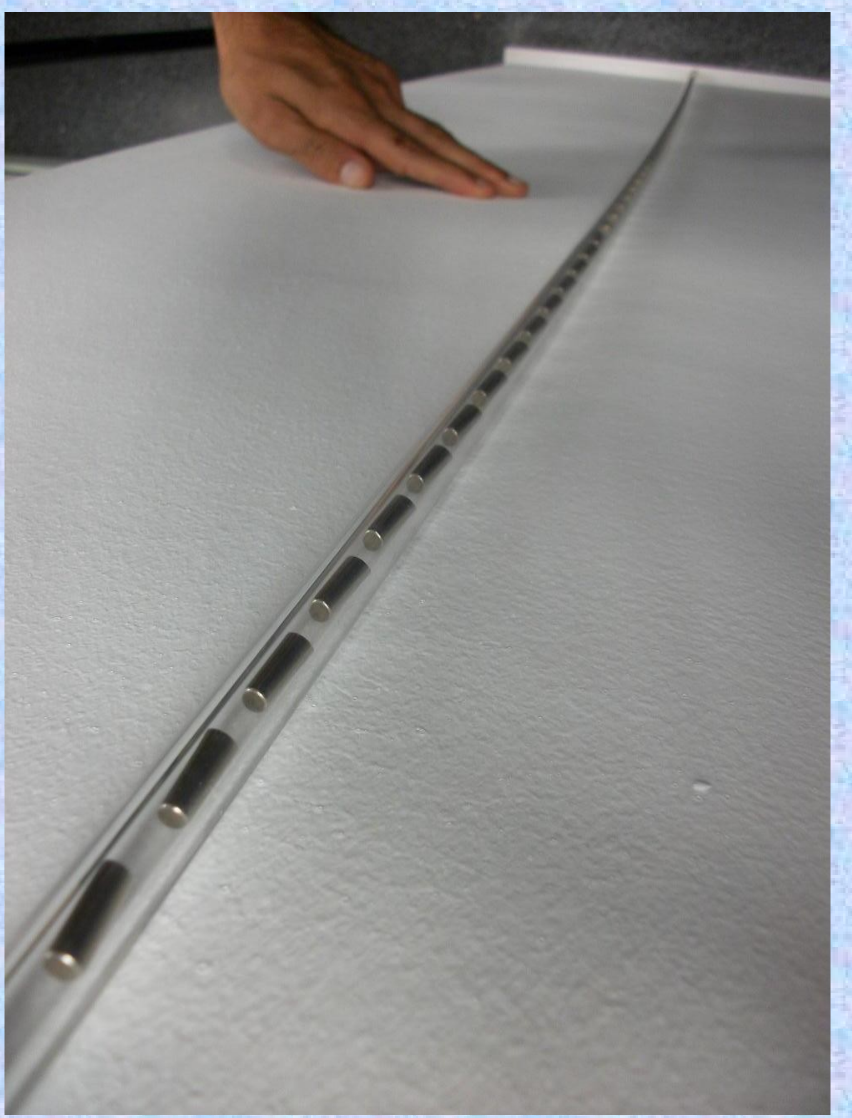
Energy profile of a kink



Kink simulation, positions



A mechanical model



Made out of magnets.
Potentials very similar to Coulomb's

Moving and static excitations

Victor Sánchez-Morcillo.
Private communication

Conclusions

- There is something energetic and localized propagating in the layers of muscovite
- A special characteristic of muscovite is that is has repulsive Coulomb’s layers
- Potassium repulsion is probably the dominant interaction in the potassium layers
- Typical FPU polynomial coupling is most likely very unsuitable for muscovite layer modelling.
- There are very energetic and localized kinks travelling in Coulomb’s chains with muscovite parameters
- Coulomb’s kinks are good candidates for quodons

References

Kosevich, Yu. A., Khomeriki, R. & Ruffo, S. (2004).
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Phys Rev E 83, 041124,1-13.

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