Radboud Universiteit Nijmegen

IN·DEI·NOMINE·FELICITER

FOM

In my element: Through the Periodic Table with pen and computer

Mikhail Katsnelson

A philosophical statement

Knowledge begins, so to speak, in the middle, and leads into the unknown - both when moving upward, and when there is a downward movement. Our goal is to gradually dissipate the darkness in both directions, and the absolute foundation - this huge elephant carrying on his mighty back the tower of truth - it exists only in a fairy tales (Hermann Weyl)

What does it mean for condensed matter physics and materials science?

Everything follows from quantum mechanics plus electrodynamics; QED is enough to explain all properties of matter around us

$$\begin{aligned} \gamma^\alpha(\partial_\alpha - ieA_\alpha)\psi + im\psi &= 0 \quad \text{where} \quad \alpha = 0, \ldots, 3 \\ F_{\alpha\beta} &= A_{\beta,\alpha} - A_{\alpha,\beta} \\ \partial^\alpha F_{\alpha\beta} &= -4\pi e j_\beta \\ \text{where} \quad j_\alpha &= \overline{\psi}\gamma_\alpha\psi. \end{aligned}$$

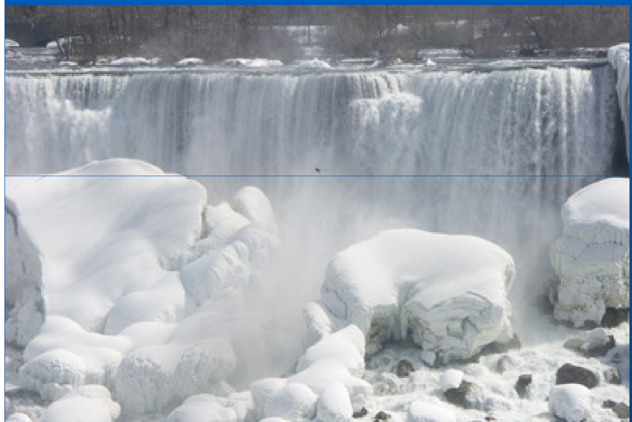
That is all. Please tell me why iridium is brittle and platinum is ductile, copper is red and silver is white, iron is ferromagnetic and vanadium is not... Not talking on biochemistry and biophysics!

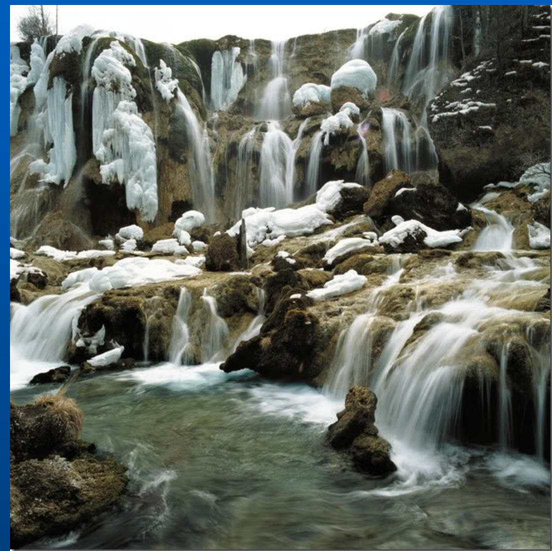
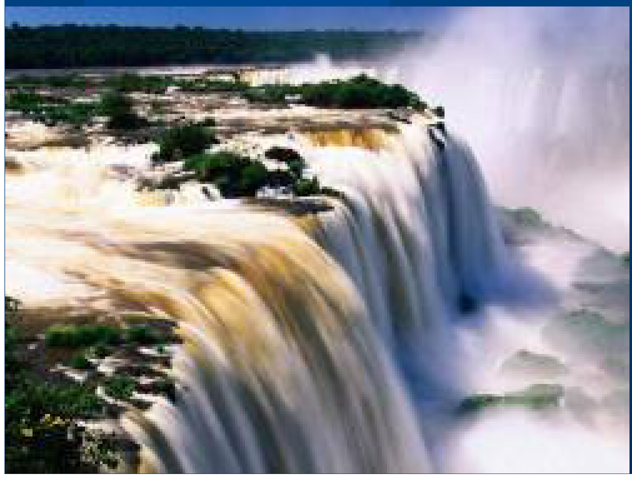
Does it help?

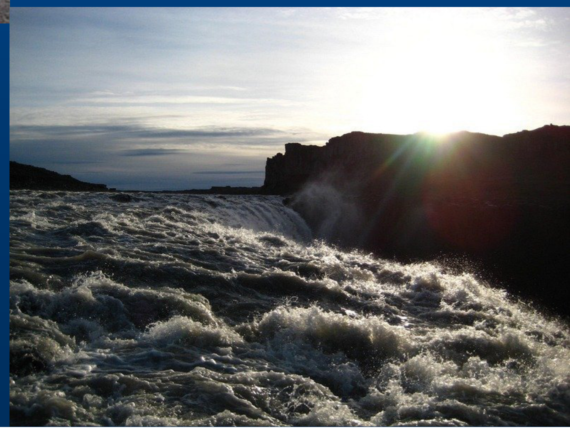
$$\nabla \cdot u = 0$$

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = f + \mu \nabla^2 u - \nabla p$$

Navier-Stocks equations:
Turbulence is here!
Can you explain this?





Is fundamental physics fundamental?

Classical thermodynamics is the only physical theory of universal content which I am convinced will never be overthrown, within the framework of applicability of its basic concepts (A. Einstein).

The laws describing our level of reality are essentially independent on the background laws. I wish our colleagues from true theory (strings, quantum gravity, etc....) all kind of success but either they will modify electrodynamics and quantum mechanics at atomic scale (and then they will be wrong) or they will not (and then I do not care). Our way is down.

How to pass from known basic laws of nature to understanding all richness and diversity of the world around us?

Pure chemical elements are already complicated enough to think very seriously

The aim of science: Understanding

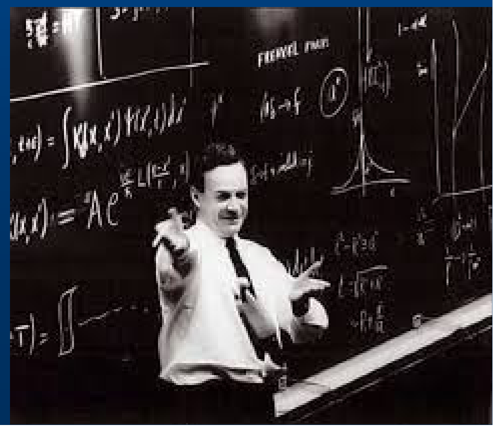
Duality of understanding and knowledge

Newton laws... Rotation...
Air resistance... I know this stuff but the result will be... well...

He does not know (?!) Newton Mechanics – but it works! He feels (=understands) what to do

I think I can safely say that nobody understands quantum mechanics

(R. P. Feynman)



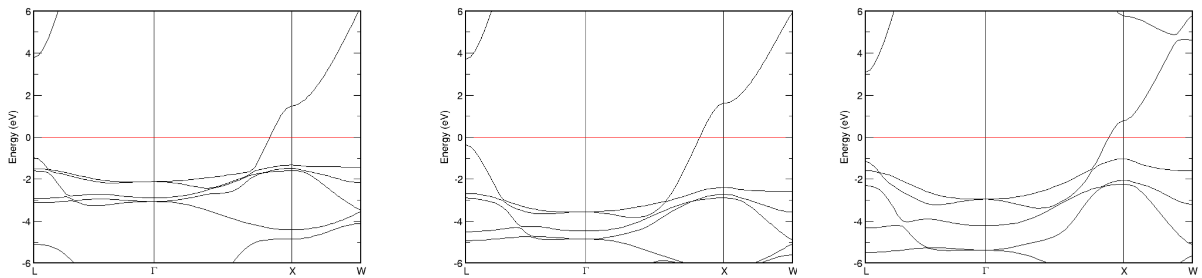
Scylla and Charybdis

Understanding "in general"

Everything is from water/fire/earth/gauge fields/quantum space-time foam/strings... and the rest is your problem.

But why silver is white, copper is red an gold is yellow?

Density functional calculations



Cu Ag Au

Taken from C. Ortiz, O. Eriksson and M. Klintenberg Comput. Mater. Sci. **44**, 1042 (2009).

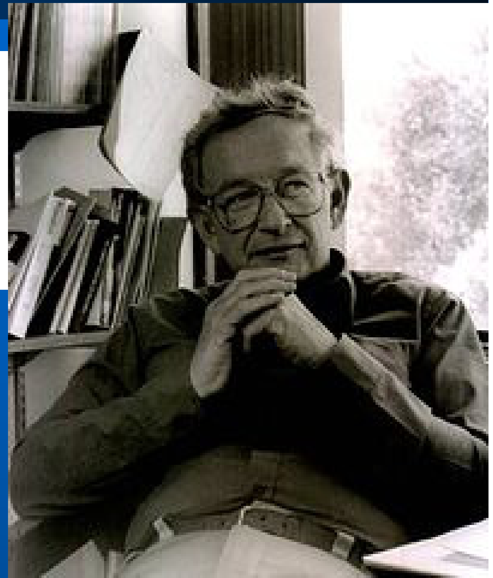
Scylla and Charybdis II

Local moments and localized states

P. W. Anderson

Reviews of Modern Physics, Vol. 50, No. 2, April 1978

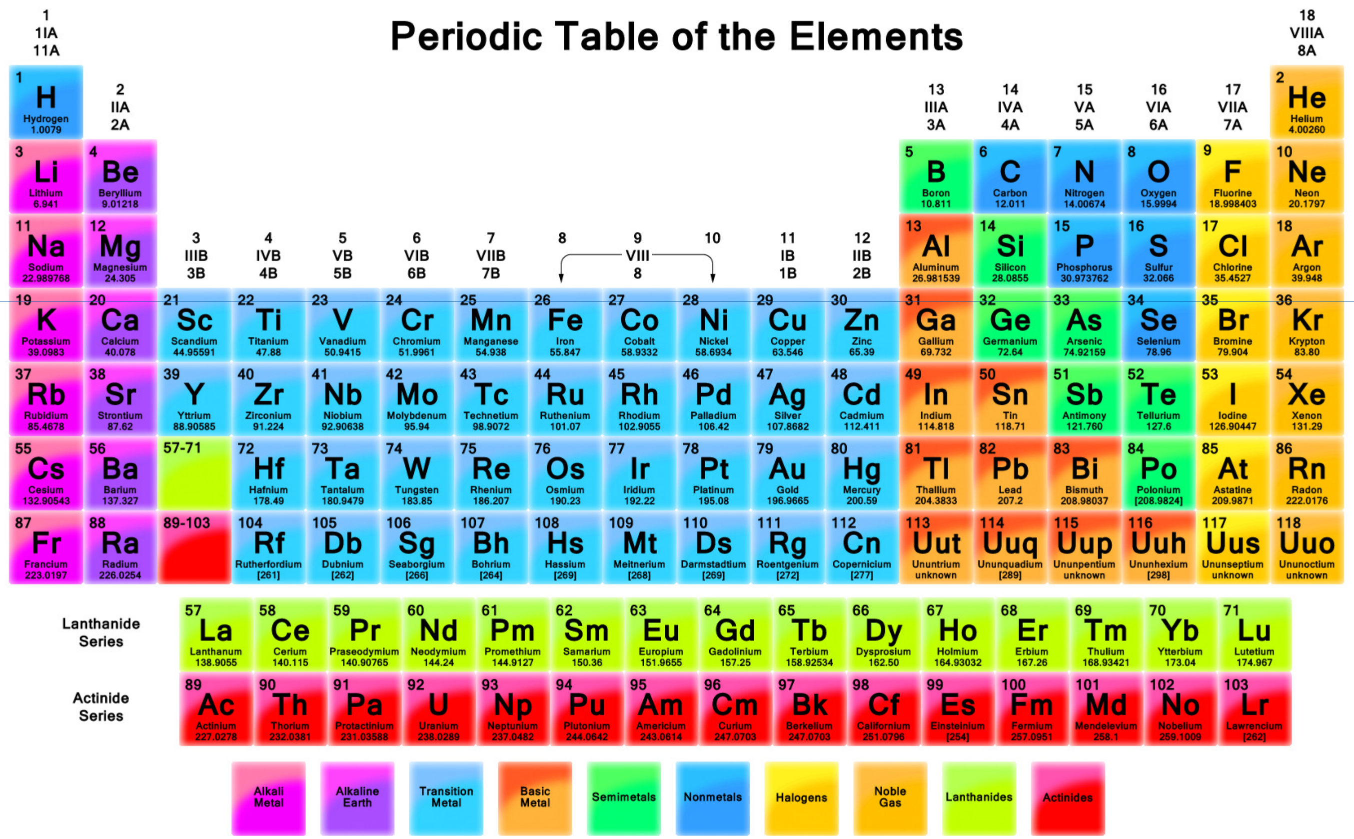
(Nobel lecture)

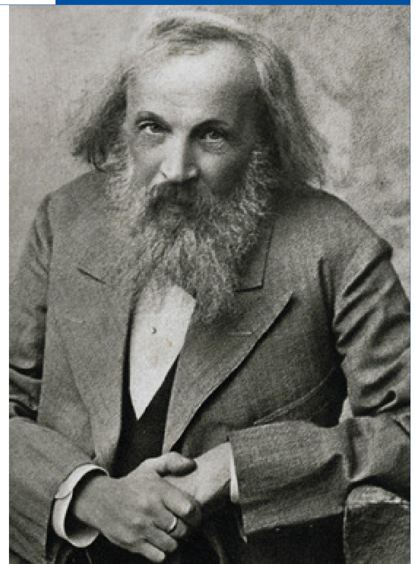


shall soon discuss. Very often such a simplified model throws more light on the real workings of nature than any number of *ab initio* calculations of individual situations, which even where correct often contain so much detail as to conceal rather than reveal reality. It can be a disadvantage rather than an advantage to be able to compute or to measure too accurately, since often what one measures or computes is irrelevant in terms of mechanism. After all, the perfect computation simply reproduces Nature, it does not explain her.

Periodic Table

Can we understand something elementary?

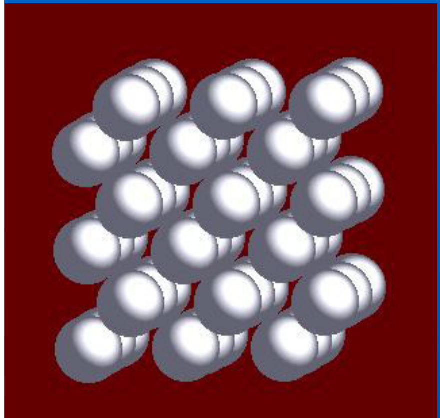




D. I. Mendeleev

An example: Alkali metals

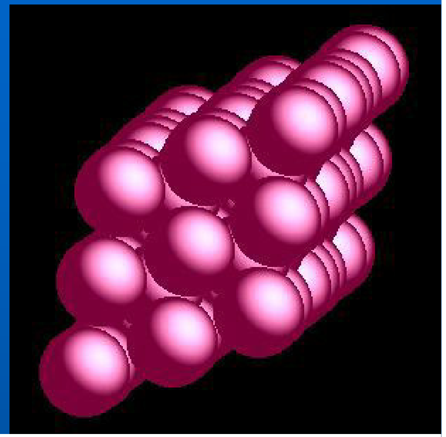
Ambient conditions: all body-centered cubic



Li, Na at low temperatures: 9R

Why? Well... Total energies are very, very close (difference ≈10^{-4})

Just numbers... Calculate!



J. Phys.: Condens. Matter 1 (1989) 5319–5335. Printed in the UK

An experimental and theoretical study of martensitic phase transitions in Li and Na under pressure

V G Vaks†, M I Katsnelson‡, V G Koreshkov‡, A I Likhtenstein§, O E Parfenov†, V F Skok‖, V A Sukhoparov‖, A V Trefilov† and A A Chernyshov†

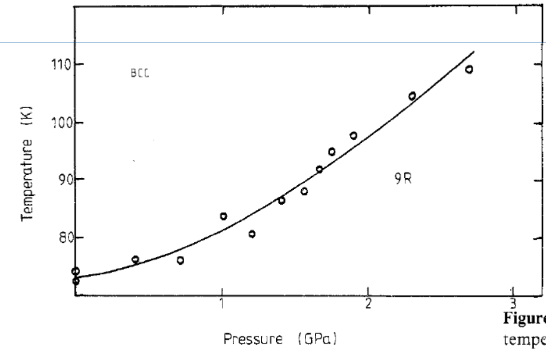


Figure 2. The martensitic transformation temperature M_s versus pressure in Li.

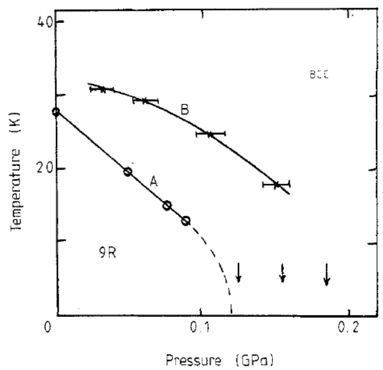
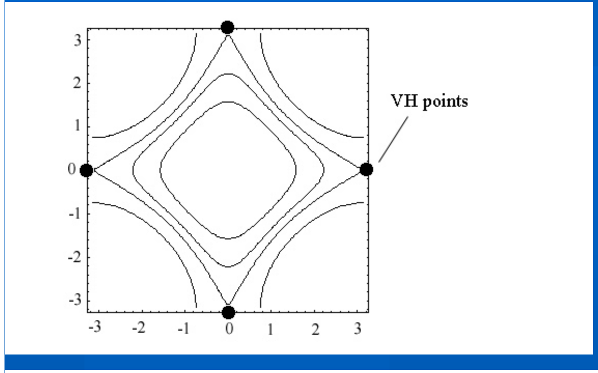


Figure 3. The martensitic transformation temperature M_s versus pressure in Na: A, the beginning of transformation, M_s, in cooling p = const; B, the beginning of transformation for decreasing pressure, T = const.

Why opposite behavior with pressure?

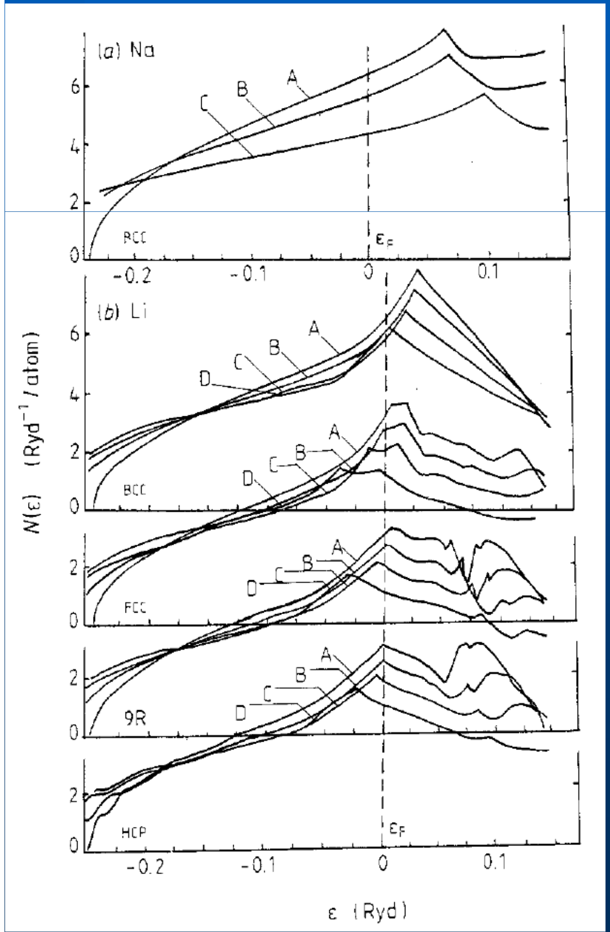
Understanding?!

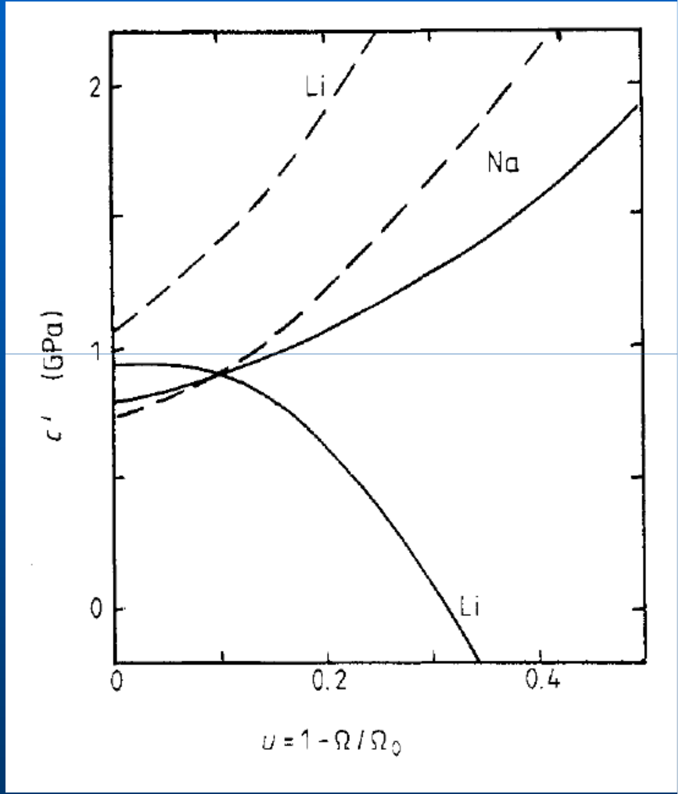


Van Hove singularities: topological property of any energy spectrum in crystals

bcc Na: away from E_F
bcc Li: towards E_F

Different role of *p*-electrons





VHS near E_F destabilize crystal structure (a general theory)

Exchange interactions and magnetism

J. Phys. F: Met. Phys. **14** (1984) L125–L128. Printed in Great Britain

LETTER TO THE EDITOR

Exchange interactions and spin-wave stiffness in ferromagnetic metals

A I Liechtenstein†, M I Katsnelson‡ and V A Gubanov†

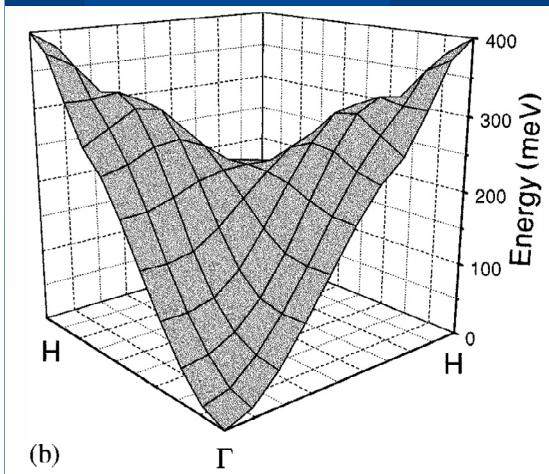
Allows to do calculations for specific materials and explain general tendencies (e.g., AFM near half-filled *d*-band)

Journal of Magnetism and Magnetic Materials 67 (1987) 65–74
North-Holland, Amsterdam

LOCAL SPIN DENSITY FUNCTIONAL APPROACH TO THE THEORY OF EXCHANGE INTERACTIONS IN FERROMAGNETIC METALS AND ALLOYS

A.I. LIECHTENSTEIN, M.I. KATSNELSON +, V.P. ANTROPOV + and V.A. GUBANOV

Basic theory to find a way to improve properties of magnetic materials



Spin-wave spectrum of iron

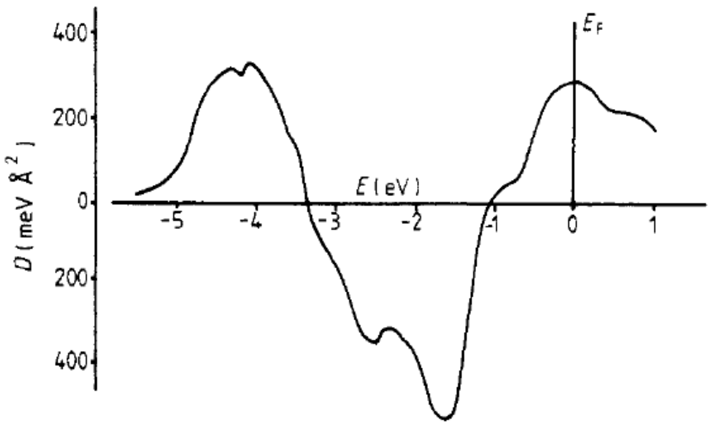


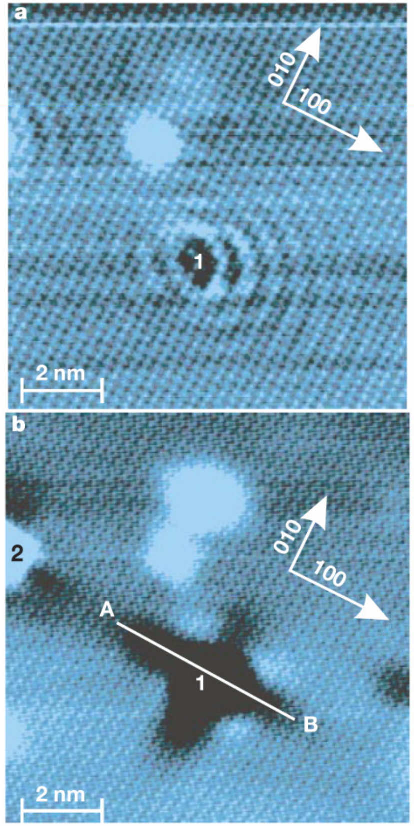
Figure 1. The spin-wave stiffness D as a function of E for ferromagnetic iron.

Orbital Kondo resonance

Real-space imaging of an orbital Kondo resonance on the Cr(001) surface

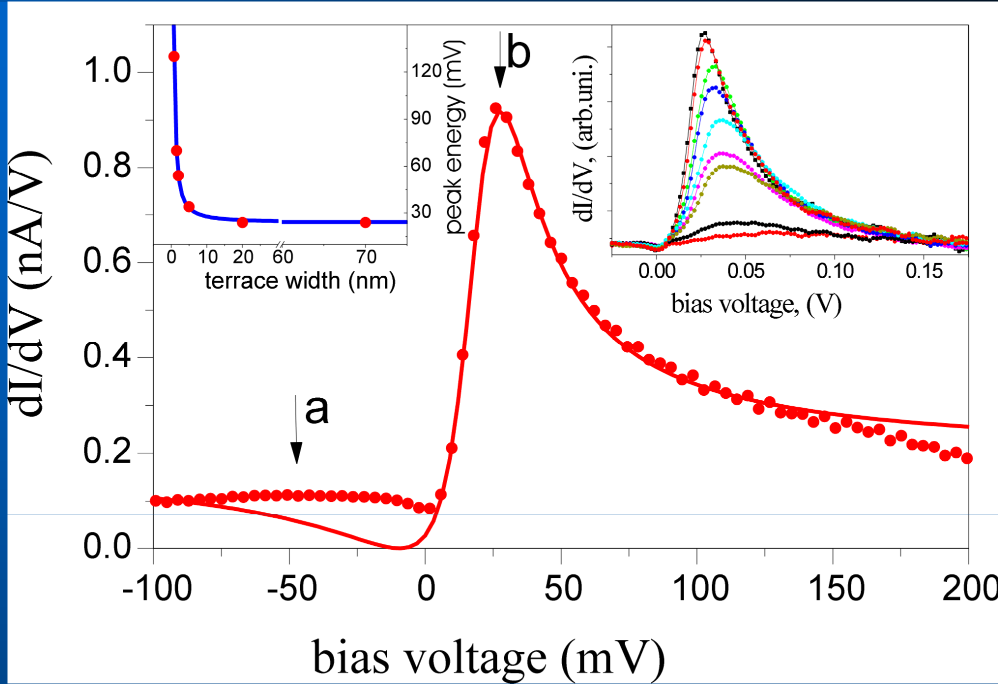
O. Yu. Kolesnychenko, R. de Kort, M. I. Katsnelson, A. I. Lichtenstein & H. van Kempen

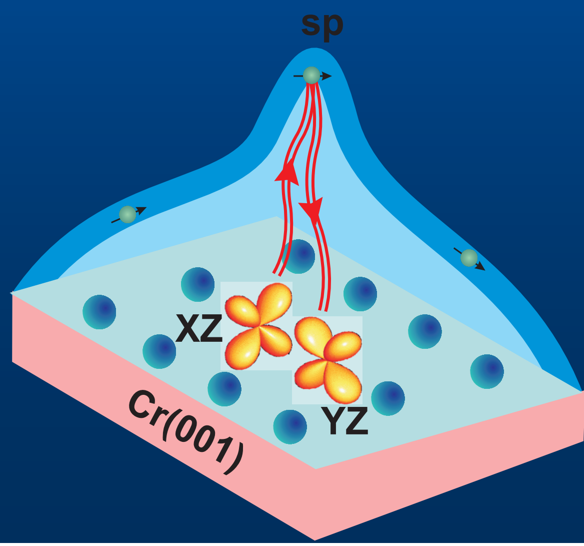
NATURE | VOL 415 | 31 JANUARY 2002



Waves from defects

«Orbital Kondo resonance»





New many-body phenomenon in pure element

From atoms to nano and mesoscale

IOP Publishing JOURNAL OF PHYSICS: CONDENSED MATTER
J. Phys.: Condens. Matter **25** (2013) 135401 (9pp) doi:10.1088/0953-8984/25/13/135401

Effect of magnetism on kinetics of γ–α transformation and pattern formation in iron

I K Razumov[1,2], Yu N Gornostyrev[1,2] and M I Katsnelson[3]

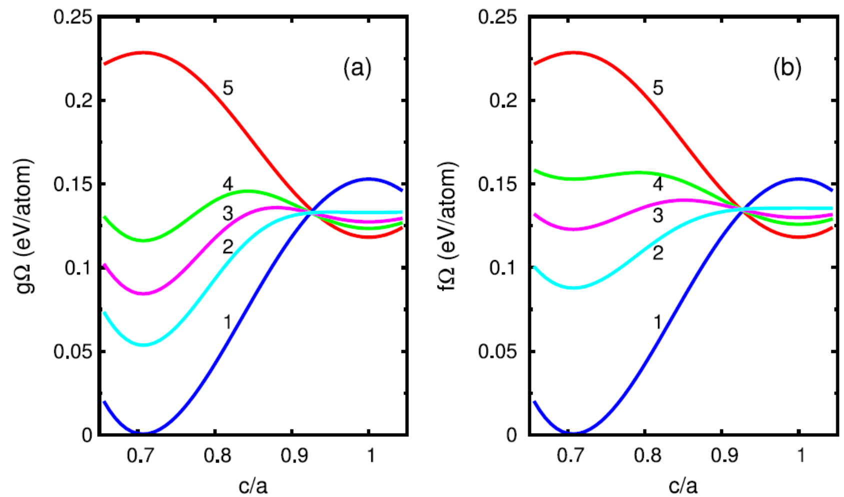
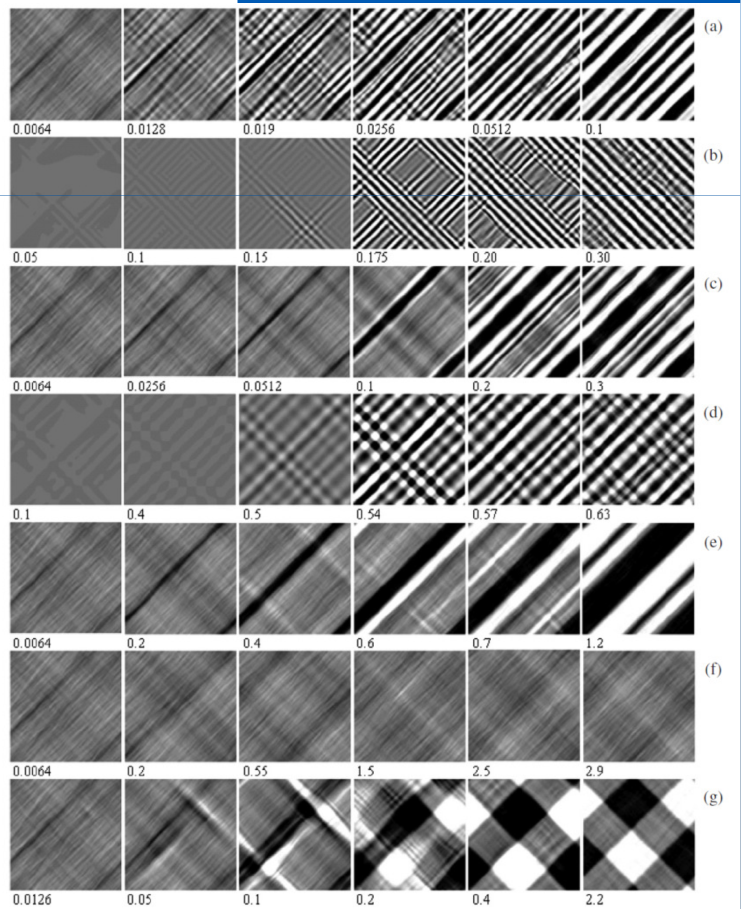


Figure 1. Energy (a) and free energy (b) as functions of tetragonal deformation for temperatures $T = 700$ K, 1000 K, 1300 K (curves 2, 3, 4, respectively) found from (5)–(8) and the first-principle computational results [22] for the Bain path in ferro- (1) and paramagnetic (5) states.



Elements are interesting

PHYSICAL REVIEW B VOLUME 62, NUMBER 12 15 SEPTEMBER 2000-II

Peculiarities of defect structure and mechanical properties of iridium: Results of *ab initio* electronic structure calculations

Yu. N. Gornostyrev,[1] M. I. Katsnelson,[1] N. I. Medvedeva,[2] O. N. Mryasov,[3] A. J. Freeman,[3] and A. V. Trefilov[4]

PRL **99,** 015901 (2007) PHYSICAL REVIEW LETTERS week ending 6 JULY 2007

Anomalous Thermal Expansion in α-Titanium

P. Souvatzis,[1] O. Eriksson,[1] and M. I. Katsnelson[2]

α-δ transition in plutonium as a Mott transition in an *f* subsystem

M. I. Katsnel'son and I. V. Solov'ev
Institute of Metal Physics, Ural Branch of the Russian Academy of Sciences, 620219, Ekaterinburg, Russia

A. V. Trefilov
I. V. Kurchatov Institute of Atomic Energy, 123482, Moscow, Russia

(Submitted 31 July 1992)
Pis'ma Zh. Eksp. Teor. Fiz. **56**, No. 5, 276–279 (10 September 1992)

Li, Na, K, Rb, Cs
Ca, Sr, Ba
Ti, Zr, Hf

Cr, Mn, Fe, Co, Ni
Ir, Rh

Sc, Y, La, Yb
Pu...

Carbon!!!

PHILOSOPHICAL MAGAZINE B, 2001, VOL. 81, NO. 12, 1893–1913

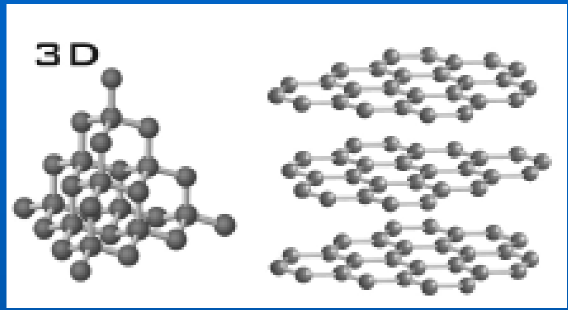
Peculiarities of anharmonic lattice dynamics and thermodynamics of alkaline-earth metals

M. I. KATSNELSON†
Institute of Metal Physics, Ekaterinburg 620219, Russia

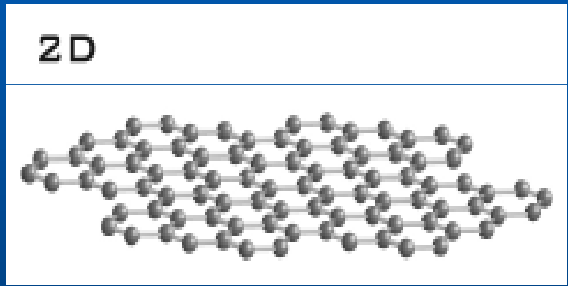
A. V. TREFILOV‡, M. N. KHLOPKIN and K. YU. KHROMOV
Russian Research Centre 'Kurchatov' Institute, Moscow 123182, Russia

Allotropes of Carbon

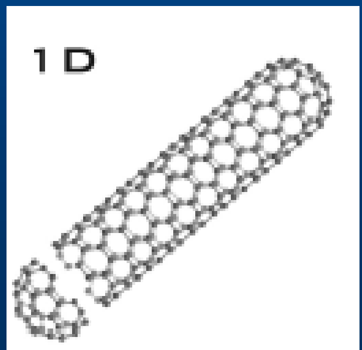
Diamond, Graphite



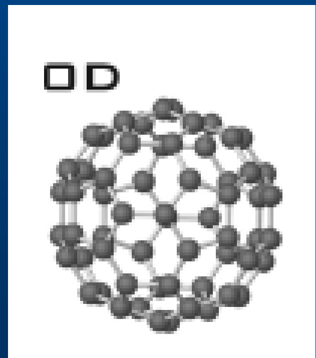
Graphene: prototype truly 2D crystal



Nanotubes

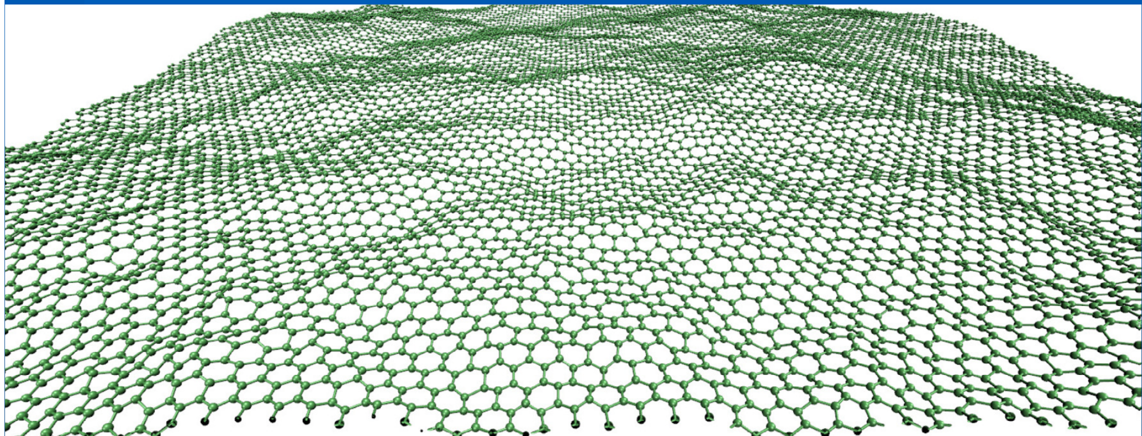


Fullerenes



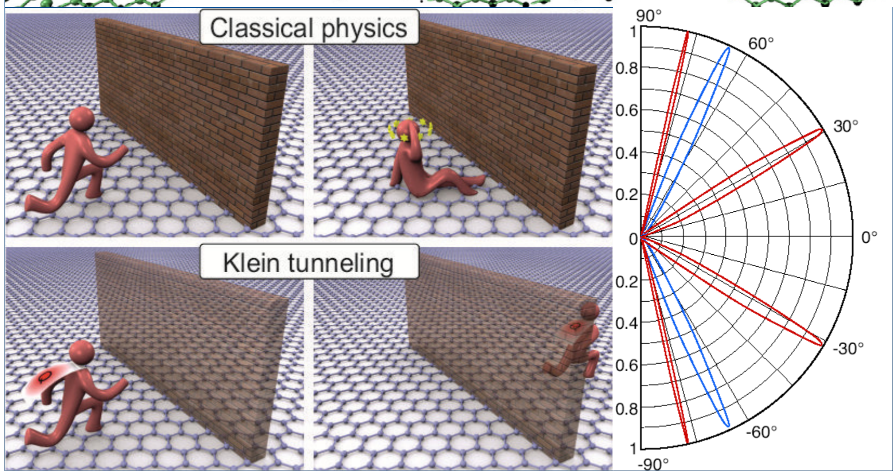
Why graphene is interesting?

1. *Applications (modern electronics is 2D, bulk is ballast)*
2. *Prototype membrane (new drosophila for 2D statistical mechanics)*
3. *CERN on the desk (mimic high energy physics)*



Ripples

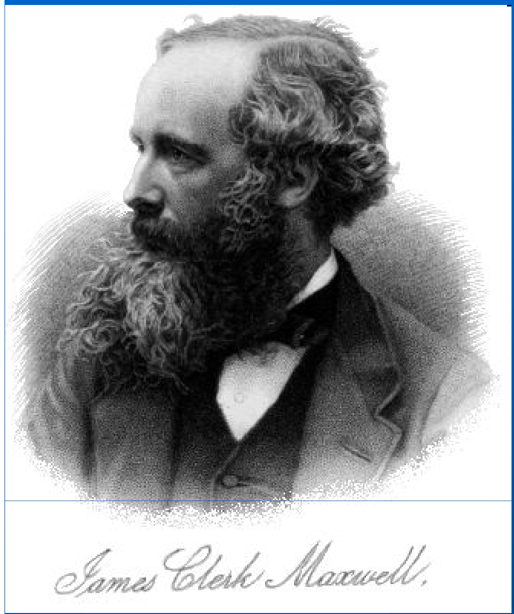
Fasolino, Los & MIK, Nature Mater. 6, 858 (2007)

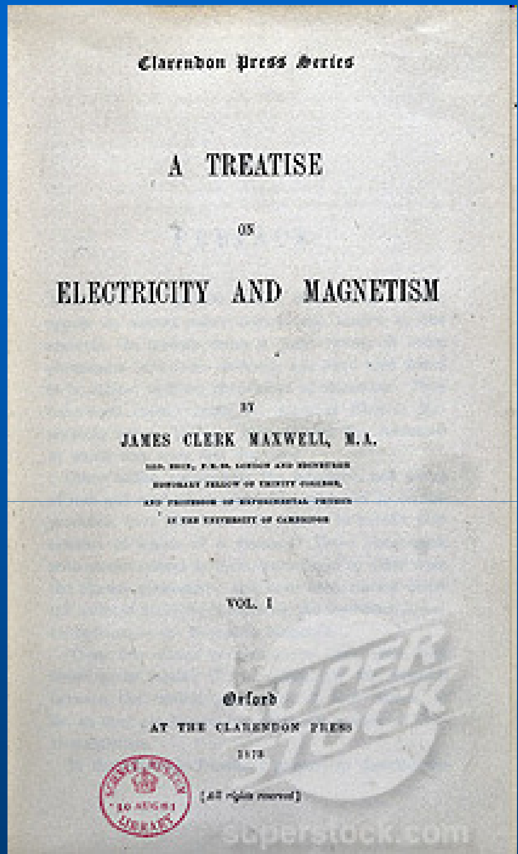


Klein tunneling

MIK, Novoselov, Geim, Nature Phys. 2, 620 (2006)

Correct theories from wrong assumptions





Clarendon Press Series

A TREATISE

ON

ELECTRICITY AND MAGNETISM

BY

JAMES CLERK MAXWELL, M.A.

VOL. I

Oxford

AT THE CLARENDON PRESS

1873

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Electromagnetic fields as deformations
in ether; gears and wheels

Also: Dirac equation... Landau theory of superfluidity of helium...

Theoretical physics as a variety of mistique experience

Beloved, believe not every spirit, but try the spirits whether they are of God (1 John 4:1)

Ye shall know them by their fruits. Do men gather grapes of thorns, or figs of thistles? (Matthew 7:16)

Fruits: to predict something correctly (like Maxwell electromagnetic waves, and then – applications)

Top pleasure and top dream for a theoretician

Graphene

1. Klein tunneling
2. Pseudomagnetic fields due to deformations
3. Relativistic collapse at a supercritical charge

Predicted and confirmed

Chiral tunnelling and the Klein paradox in graphene

M. I. KATSNELSON[1]*, K. S. NOVOSELOV[2] AND A. K. GEIM[2]*

nature physics | VOL 2 | SEPTEMBER 2006

nature physics LETTERS
PUBLISHED ONLINE: 1 FEBRUARY 2009 | DOI: 10.1038/NPHYS1198

Quantum interference and Klein tunnelling in graphene heterojunctions

Andrea F. Young and Philip Kim*

LETTERS nature physics
PUBLISHED ONLINE: 27 SEPTEMBER 2009 | DOI: 10.1038/NPHYS1420

Energy gaps and a zero-field quantum Hall effect in graphene by strain engineering

F. Guinea[1]*, M. I. Katsnelson[2] and A. K. Geim[3]*

Strain-Induced Pseudo–Magnetic Fields Greater Than 300 Tesla in Graphene Nanobubbles

N. Levy,[1,2]*† S. A. Burke,[1]*‡ K. L. Meaker,[1] M. Panlasigui,[1] A. Zettl,[1,2] F. Guinea,[3] A. H. Castro Neto,[4] M. F. Crommie[1,2]§

30 JULY 2010 VOL 329 SCIENCE

PRL 99, 236801 (2007) PHYSICAL REVIEW LETTERS week ending 7 DECEMBER 2007

Vacuum Polarization and Screening of Supercritical Impurities in Graphene

A. V. Shytov,[1] M. I. Katsnelson,[2] and L. S. Levitov[3]

PRL 99, 246802 (2007) PHYSICAL REVIEW LETTERS week ending 14 DECEMBER 2007

Atomic Collapse and Quasi–Rydberg States in Graphene

A. V. Shytov,[1] M. I. Katsnelson,[2] and L. S. Levitov[3]

Observing Atomic Collapse Resonances in Artificial Nuclei on Graphene

Yang Wang,[1,2]* Dillon Wong,[1,2]* Andrey V. Shytov,[3] Victor W. Brar,[1,2] Sangkook Choi,[1] Qiong Wu,[1,2] Hsin-Zon Tsai,[1] William Regan,[1,2] Alex Zettl,[1,2] Roland K. Kawakami,[5] Steven G. Louie,[1,2] Leonid S. Levitov,[4] Michael F. Crommie[1,2]†

10 MAY 2013 VOL 340 SCIENCE

Plans

To combine studies of particular systems (graphene, iron...) with general concepts

- Many-body theory of graphene

- Statistical mechanics of membranes

- Pattern formation and the origin of physical and chemical complexity

- Magnetism out of equilibrium

Many thanks!!!

To NWO for this sign of recognition and opportunity to do further really interesting science (which will be useful)

To my friends, colleagues, collaborators, coauthors, teachers and pupils

To Radboud University, Faculty of Science, Institute for Molecules and Materials for wonderful environment and support

To FOM for support

And thank you for your attention