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

Mikhail Katsnelson
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.

\[
\gamma^\alpha (\partial_\alpha - ieA_\alpha)\psi + im\psi = 0 \quad \text{where} \quad \alpha = 0, \ldots, 3
\]

\[
F_{\alpha\beta} = A_{\beta,\alpha} - A_{\alpha,\beta}
\]

\[
\partial^\alpha F_{\alpha\beta} = -4\pi e j_\beta
\]

where \( j_\alpha = \overline{\psi} \gamma_\alpha \psi \).

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

\[ \nabla \cdot u = 0 \]

\[ \frac{\partial u}{\partial t} + u \cdot \nabla u = f + \mu \nabla^2 u - \nabla p \]
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 and gold is yellow?

Density functional calculations

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.
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 $\approx 10^{-4}$)

Just numbers... Calculate!

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†

Why opposite behavior with pressure?

Figure 2. The martensitic transformation temperature $M$, versus pressure in Li.

Figure 3. The martensitic transformation temperature $M$, versus pressure in Na: A, the beginning of transformation, $M_A$ in cooling $p = \text{const}$; B, the beginning of transformation for decreasing pressure, $T = \text{const}$. 
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


LETTER TO THE EDITOR

Exchange interactions and spin-wave stiffness in ferromagnetic metals

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

Spin-wave spectrum of iron

Figure 1. The spin-wave stiffness $D$ as a function of $E$ for ferromagnetic iron.
Real-space imaging of an orbital Kondo resonance on the Cr(001) surface

Waves from defects

New many-body phenomenon in pure element
Effect of magnetism on kinetics of $\gamma-\alpha$ 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

Peculiarities of defect structure and mechanical properties of iridium: Results of \textit{ab initio} electronic structure calculations


Anomalous Thermal Expansion in $\alpha$-Titanium
P. Souvatzis, O. Eriksson, and M. I. Katsnelson

$\alpha$-$\delta$ transition in plutonium as a Mott transition in an $f$ subsystem
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(Submitted 31 July 1992)

Li, Na, K, Rb, Cs
Ca, Sr, Ba
Ti, Zr, Hf
Cr, Mn, Fe, Co, Ni
Ir, Rh

Peculiarities of anharmonic lattice dynamics and thermodynamics of alkaline-earth metals
M. I. Katsnelson
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Sc, Y, La, Yb
Pu... Carbon!!!
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
Correct theories from wrong assumptions

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. Katsnelson¹*, K. S. Novoselov² and A. K. Geim²*

Quantum interference and Klein tunnelling in graphene heterojunctions

Andrea F. Young and Philip Kim*

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

F. Guinea¹*, M. I. Katsnelson² and A. K. Geim³*

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

N. Levy,¹,²† S. A. Burke,¹,²† K. L. Meaker,¹ M. Panlasigui,³ A. Zettl,¹,² F. Guinea,³ A. H. Castro Neto,⁴ M. F. Crommie¹,²,5

Vacuum Polarization and Screening of Supercritical Impurities in Graphene

A. V. Shytov,¹ M. I. Katsnelson,³ and L. S. Levitov⁵

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. Crommie¹,²,‡
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

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