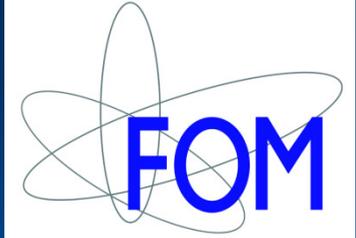


Radboud Universiteit Nijmegen

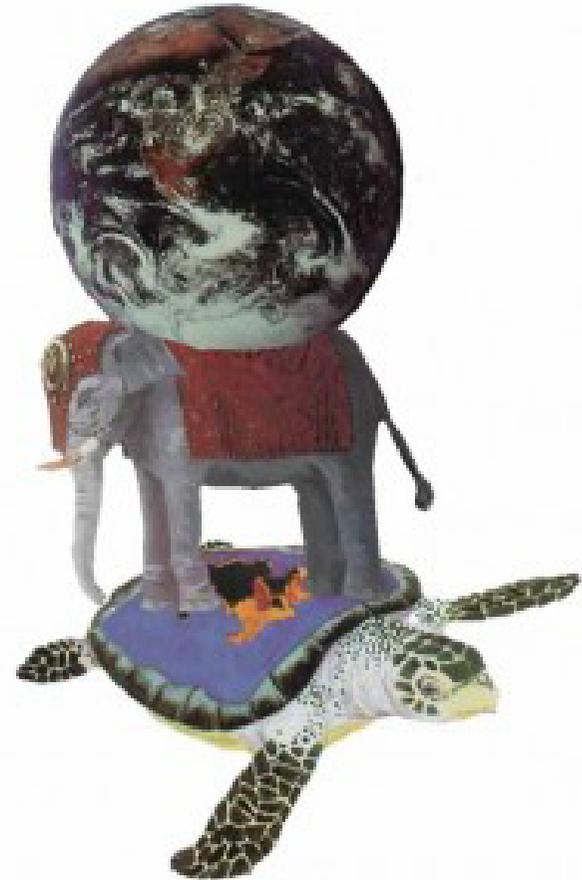


*In my element:
Through the Periodic
Table
with pen and computer*

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

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

$$F_{\alpha\beta} = A_{\beta,\alpha} - A_{\alpha,\beta}$$

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

$$\text{where} \quad j_\alpha = \bar{\psi}\gamma_\alpha\psi.$$

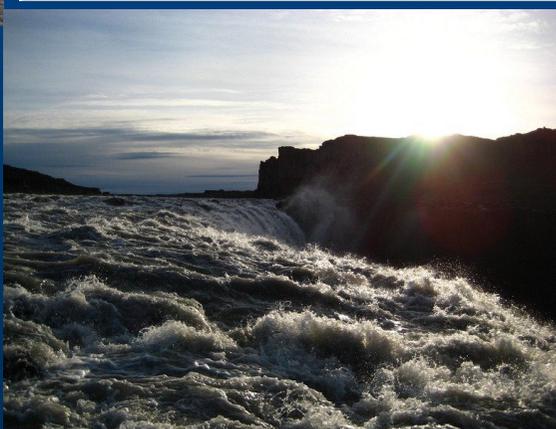
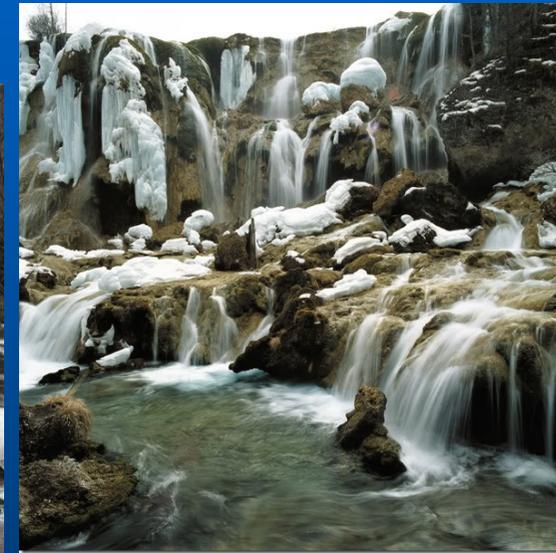
That is all. Please tell me why iridium is brittle and platinum is ductile, copper is red and silver is white, iron is ferromagnetic and vanadium is not... Not talking on biochemistry and biophysics!

Does it help?

$$\nabla \cdot u = 0$$

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

Navier-Stokes 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

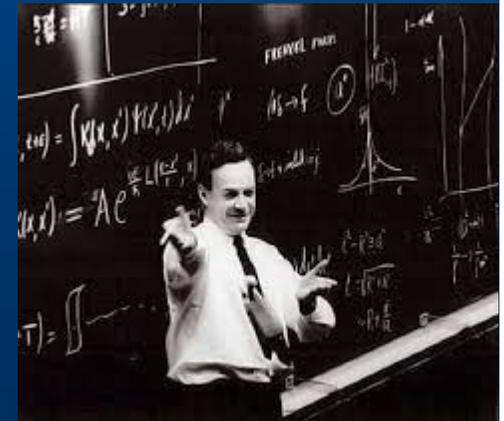
Duality of understanding and knowledge



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)**



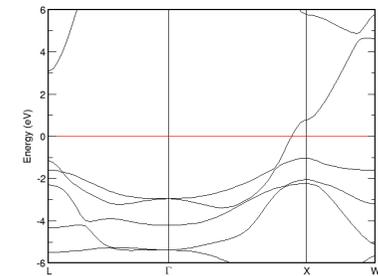
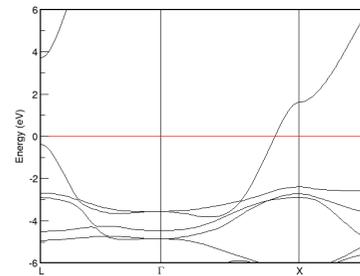
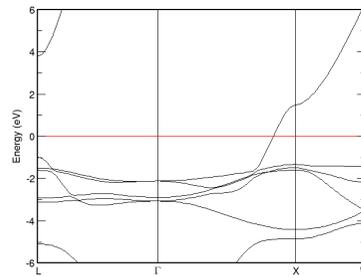
Scylla and Charybdis



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 and gold is yellow?

Density functional calculations



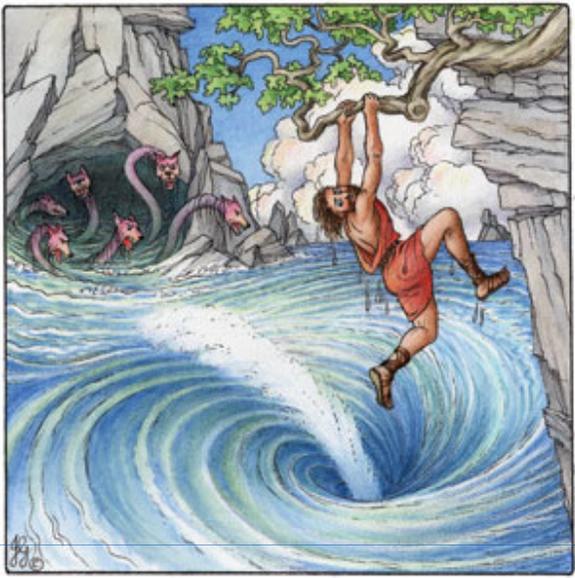
Cu

Ag

Au

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

Scylla and Charybdis II

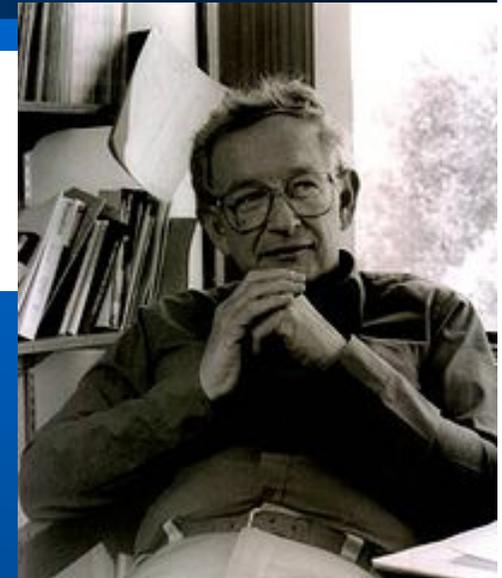


Local moments and localized states

P. W. Anderson

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

(Nobel lecture)



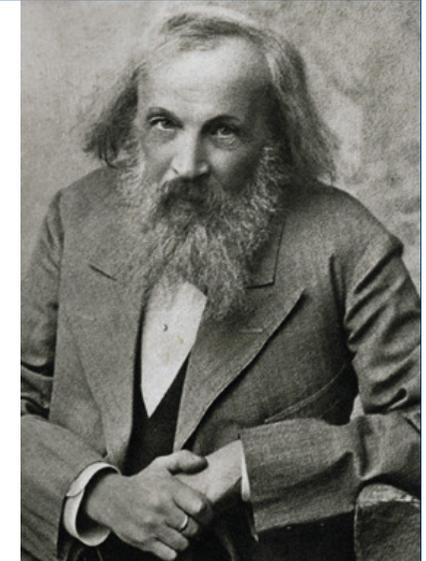
shall soon discuss. Very often such a simplified model throws more light on the real workings of nature than any number of *ab initio* calculations of individual situations, which even where correct often contain so much detail as to conceal rather than reveal reality. It can be a disadvantage rather 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?

Periodic Table of the Elements

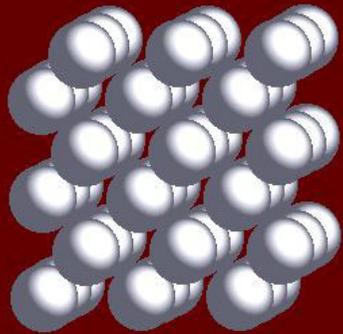
1 1IA 11A																	18 VIIIA 8A		
1 H Hydrogen 1.0079			2 IIA 2A											13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	2 He Helium 4.00260
3 Li Lithium 6.941			4 Be Beryllium 9.01218											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.00574	8 O Oxygen 15.9994	9 F Fluorine 18.998403	10 Ne Neon 20.1797
11 Na Sodium 22.989768			12 Mg Magnesium 24.305	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 8	10 VIII 8	11 IB 1B	12 IIB 2B	13 Al Aluminum 26.981539	14 Si Silicon 28.0855	15 P Phosphorus 30.973762	16 S Sulfur 32.066	17 Cl Chlorine 35.4527	18 Ar Argon 39.948
19 K Potassium 39.0983			20 Ca Calcium 40.078	21 Sc Scandium 44.95591	22 Ti Titanium 47.88	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938	26 Fe Iron 55.847	27 Co Cobalt 58.9332	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.732	32 Ge Germanium 72.64	33 As Arsenic 74.92159	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.80
37 Rb Rubidium 85.4678			38 Sr Strontium 87.62	39 Y Yttrium 88.90585	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.94	43 Tc Technetium 98.9072	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.9055	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.90447	54 Xe Xenon 131.29
55 Cs Cesium 132.90543			56 Ba Barium 137.327	57-71 Lanthanide Series	72 Hf Hafnium 178.49	73 Ta Tantalum 180.9479	74 W Tungsten 183.85	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.9665	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.98037	84 Po Polonium [208.9824]	85 At Astatine 209.9871	86 Rn Radon 222.0176
87 Fr Francium 223.0197			88 Ra Radium 226.0254	89-103 Actinide Series	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Uuq Ununquadium [289]	115 Uup Ununpentium unknown	116 Uuh Ununhexium [298]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown
				57 La Lanthanum 138.9055	58 Ce Cerium 140.115	59 Pr Praseodymium 140.90765	60 Nd Neodymium 144.24	61 Pm Promethium 144.9127	62 Sm Samarium 150.36	63 Eu Europium 151.9655	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92534	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93032	68 Er Erbium 167.26	69 Tm Thulium 168.93421	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967	
				89 Ac Actinium 227.0278	90 Th Thorium 232.0381	91 Pa Protactinium 231.03888	92 U Uranium 238.0289	93 Np Neptunium 237.0482	94 Pu Plutonium 244.0642	95 Am Americium 243.0614	96 Cm Curium 247.0703	97 Bk Berkelium 247.0703	98 Cf Californium 251.0796	99 Es Einsteinium [254]	100 Fm Fermium 257.0951	101 Md Mendelevium 258.1	102 No Nobelium 259.1009	103 Lr Lawrencium [262]	
				Alkali Metal	Alkaline Earth	Transition Metal	Basic Metal	Semimetals	Nonmetals	Halogens	Noble Gas	Lanthanides	Actinides						



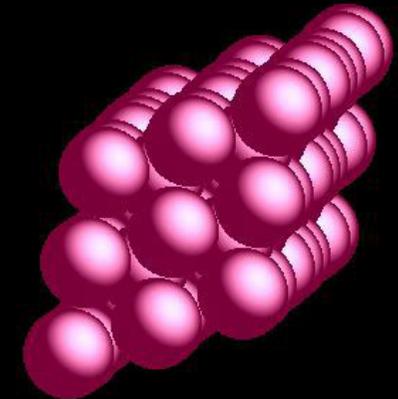
D. I. Mendeleev

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!



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[†]

Why opposite behavior
with pressure?

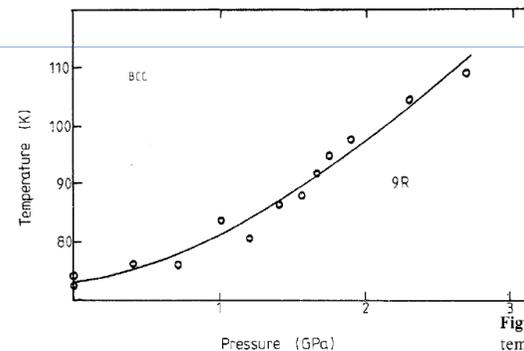


Figure 2. The martensitic transformation temperature M_s versus pressure in Li.

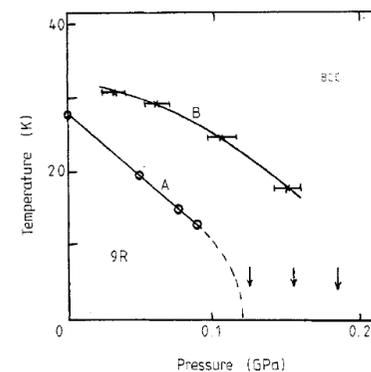
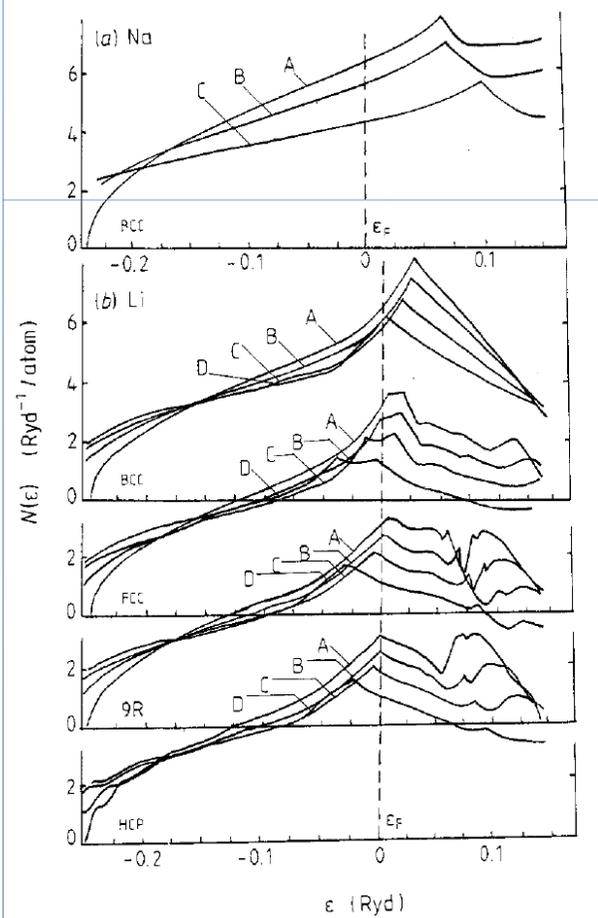
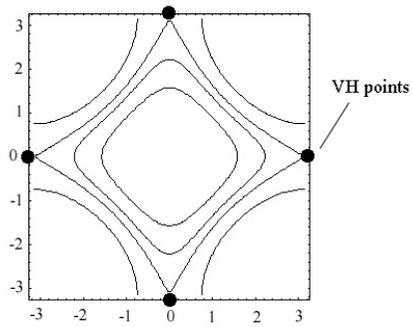


Figure 3. The martensitic transformation temperature M_s versus pressure in Na: A, the beginning of transformation, M_s , in cooling $p = \text{const}$; B, the beginning of transformation for decreasing pressure, $T = \text{const}$.

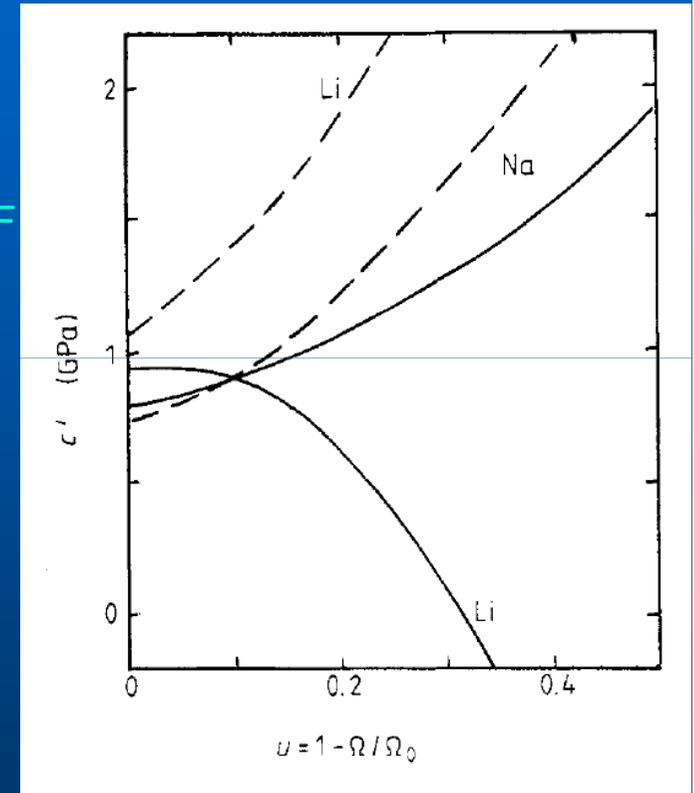
Understanding?!

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

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[†]

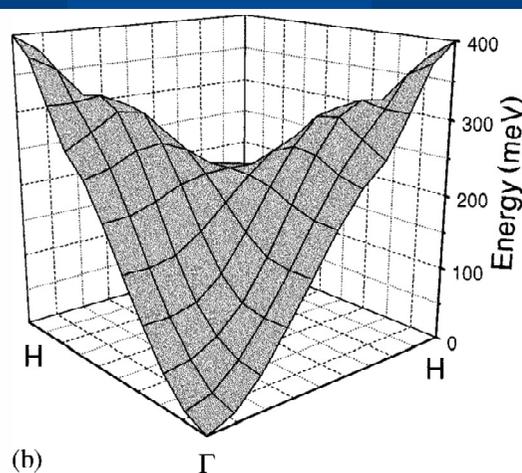
Journal of Magnetism and Magnetic Materials 67 (1987) 65–74
North-Holland, Amsterdam

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

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

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



Spin-wave spectrum of iron

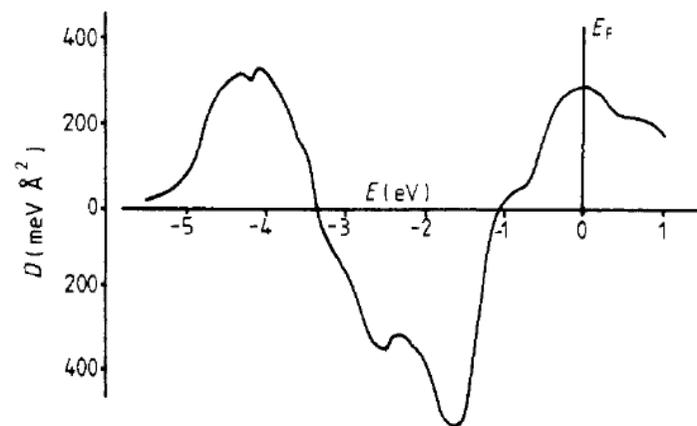


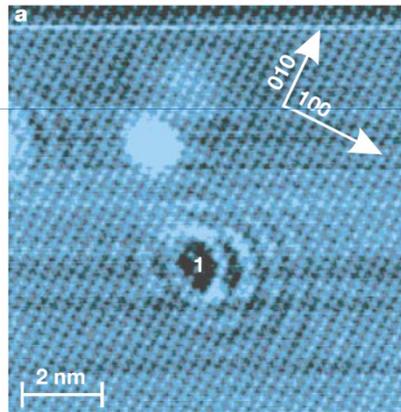
Figure 1. The spin-wave stiffness D as a function of E for ferromagnetic iron.

Orbital Kondo resonance

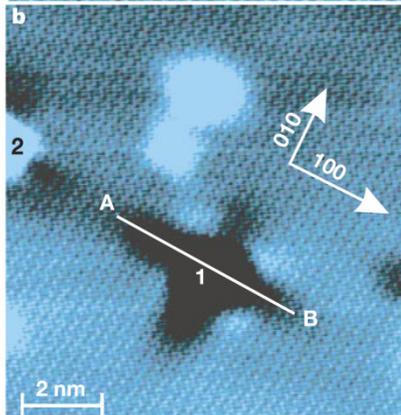
Real-space imaging of an orbital Kondo resonance on the Cr(001) surface

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

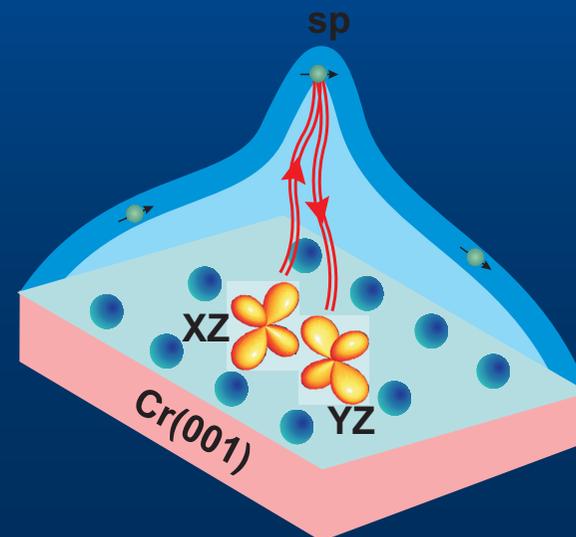
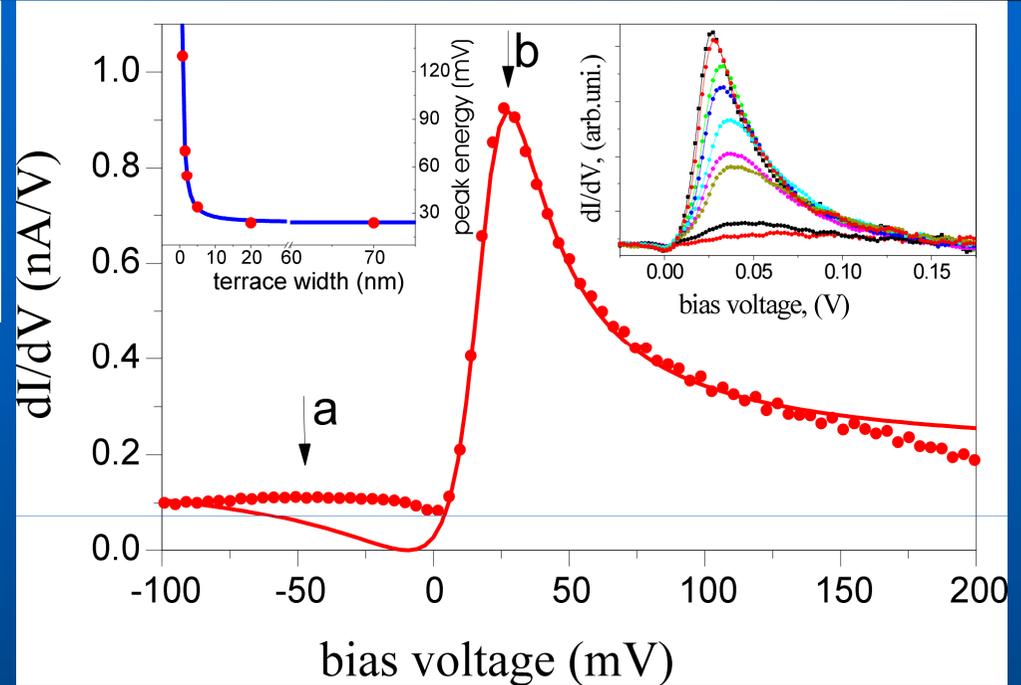
NATURE | VOL 415 | 31 JANUARY 2002



Waves from defects



«Orbital Kondo resonance»



New many-body phenomenon in pure element

From atoms to nano and mesoscale

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 Katsnelson³

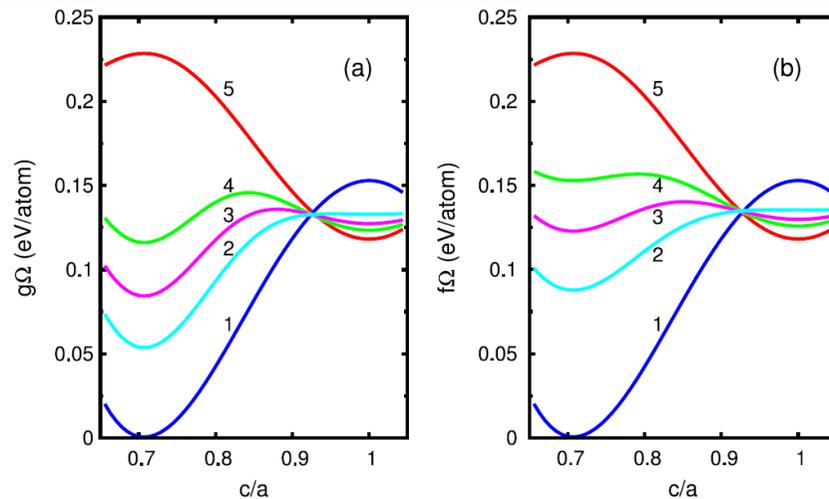
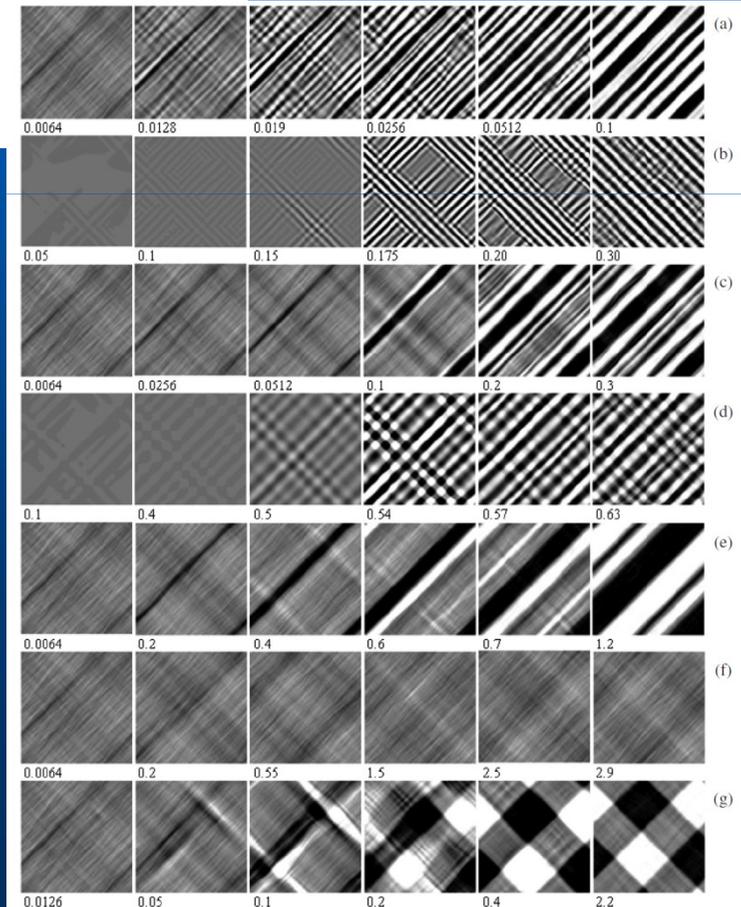


Figure 1. Energy (a) and free energy (b) as functions of tetragonal deformation for temperatures $T = 700$ K, 1000 K, 1300 K (curves 2, 3, 4, respectively) found from (5)–(8) and the first-principle computational results [22] for the Bain path in ferro- (1) and paramagnetic (5) states.



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. Trefilov⁴

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. Katsnelson²

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)

Sc, Y, La, Yb
Pu...

Carbon!!!

Li, Na, K, Rb, Cs

Ca, Sr, Ba

Ti, Zr, Hf

Cr, Mn, Fe, Co, Ni

Ir, Rh

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



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

M. I. KATSNELSON†

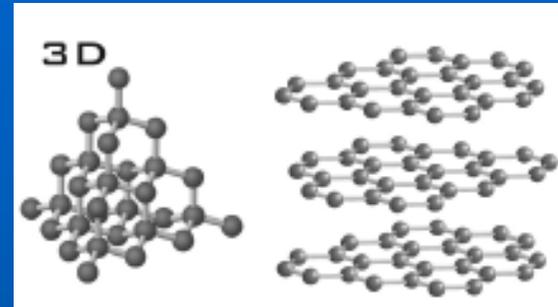
Institute of Metal Physics, Ekaterinburg 620219, Russia

A. V. TREFILOV‡, M. N. KHLOPKIN and K. YU. KHROMOV

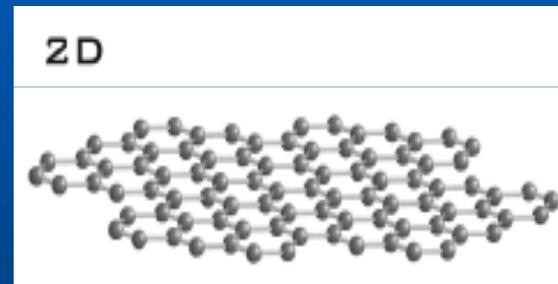
Russian Research Centre 'Kurchatov' Institute, Moscow 123182, Russia

Allotropes of Carbon

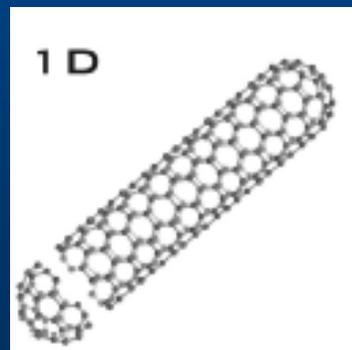
Diamond, Graphite



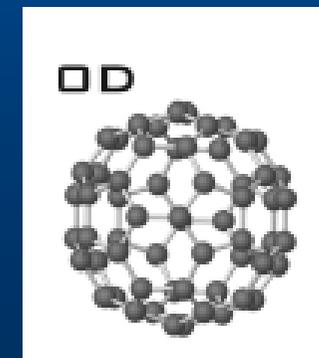
Graphene: prototype
truly 2D crystal



Nanotubes

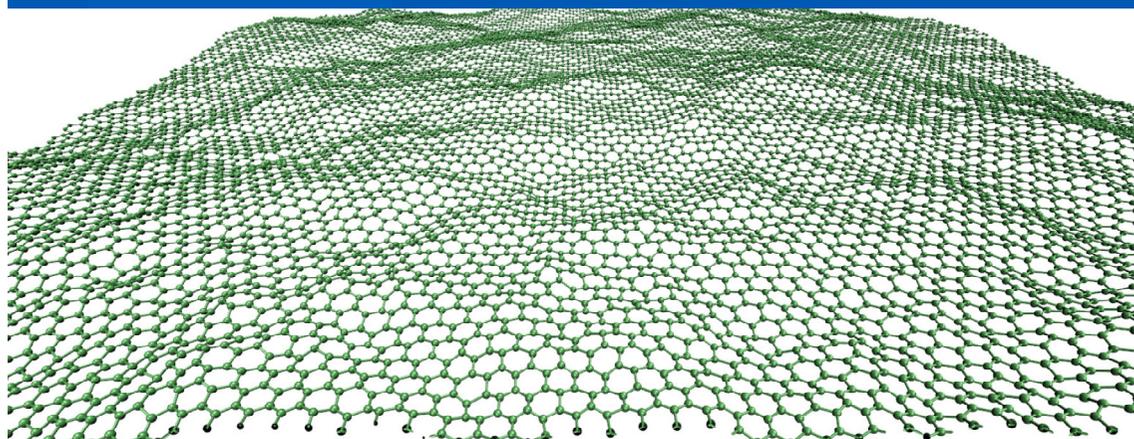


Fullerenes



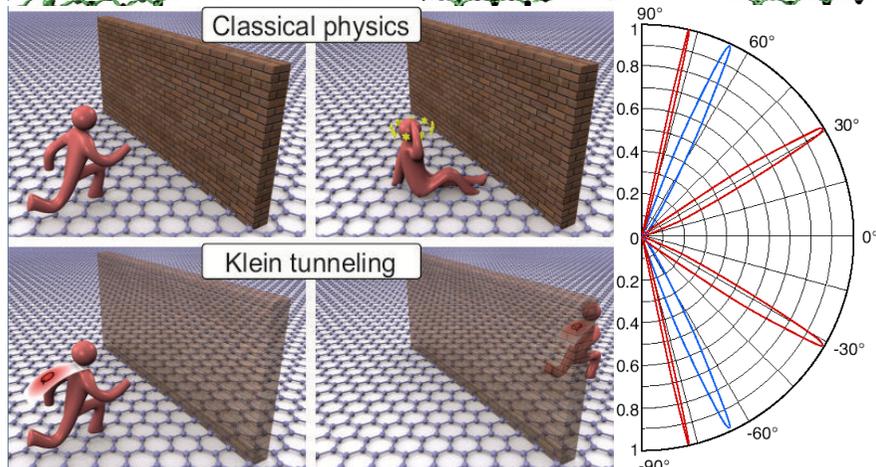
Why graphene is interesting?

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)



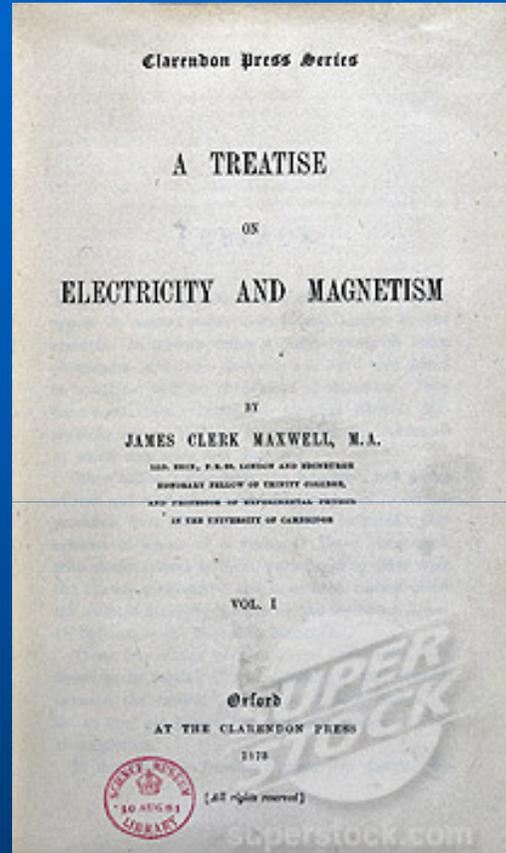
Klein tunneling

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

Correct theories from wrong assumptions



James Clerk Maxwell.



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. NOVOSELOV² AND A. K. GEIM^{2*}

nature physics | VOL 2 | SEPTEMBER 2006

LETTERS

PUBLISHED ONLINE: 27 SEPTEMBER 2009 | DOI: 10.1038/NPHYS1420

nature
physics

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

F. Guinea^{1*}, M. I. Katsnelson² and A. K. Geim^{3*}

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^{*}

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. Levitov³

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. Levitov³

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