Radboud Universiteit

UPPSALA UNIVERSITET

From quantum many-body physics to materials and sustainability

Mikhail Katsnelson

WISE Guest Professor Lecture, 6 November 2025

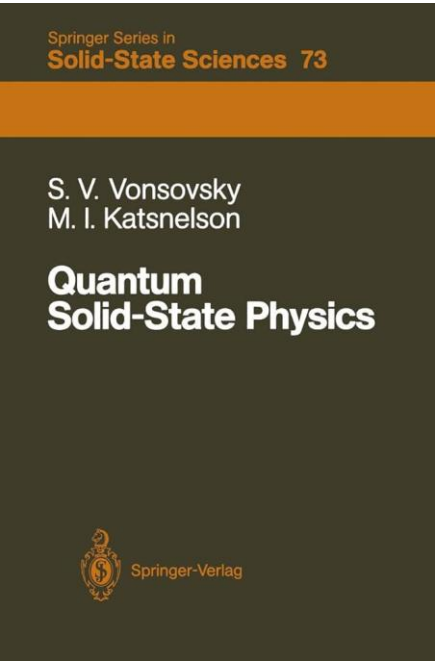
erc Synergy Grant

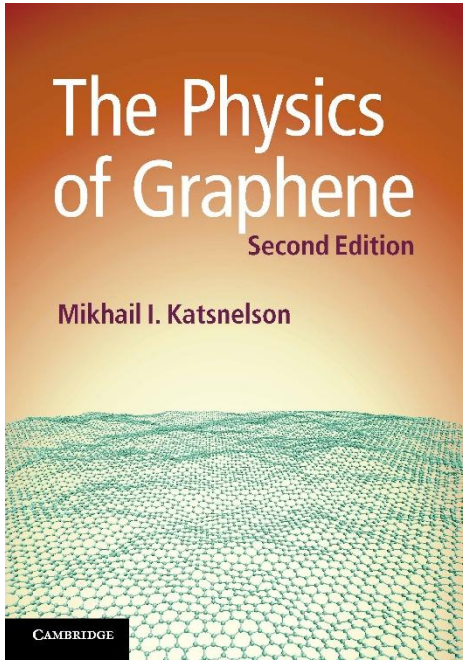
Wallenberg Initiative Materials Science for Sustainability

What I am doing as a materials scientist?

(1) Graphene and other 2D materials
(2) Theoretical and computational magnetism
(3) Electronic structure of strongly correlated materials

Also core-level spectroscopy, anharmonic lattice dynamics, phase transformations in solids, rare earths, actinides, iron and steel…





Selected Reviews

REVIEWS OF MODERN PHYSICS, VOLUME 80, JANUARY–MARCH 2008

Half-metallic ferromagnets: From band structure to many-body effects

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REVIEWS OF MODERN PHYSICS, VOLUME 95, JULY–SEPTEMBER 2023

Quantitative theory of magnetic interactions in solids

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Physics Reports 496 (2010) 109–148

Contents lists available at ScienceDirect

Physics Reports

journal homepage: www.elsevier.com/locate/physrep

Gauge fields in graphene

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REVIEWS OF MODERN PHYSICS, VOLUME 90, APRIL–JUNE 2018

Diagrammatic routes to nonlocal correlations beyond dynamical mean field theory

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Graphene: 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
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. 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

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!

Quantum Hamiltonians: General

In condensed matter physics we know the basic laws, it is laws of quantum mechanics

Time-dependent Schrödinger equation *(general)*

$$i\hbar\frac{\partial}{\partial t}|\Psi(\mathbf{r},t)\rangle = \hat{H}|\Psi(\mathbf{r},t)\rangle$$

In solids/liquids/molecules/clusters...

$$\hat{H} = \hat{T}_n + V_{nn}\left(\vec{R}_l\right) + \hat{H}_e\left(\vec{R}_l\right)$$

$$\hat{T}_n = \sum_l \frac{\hat{\vec{P}}_l^2}{2M_l}$$ **Kinetic energy of nuclei**

$$V_{nn}\left(\vec{R}_l\right) = \frac{1}{2}\sum_{l\neq l'}\frac{Z_l Z_{l'} e^2}{\left|\vec{R}_l - \vec{R}_{l'}\right|}$$ **Coulomb repulsion of nuclei**

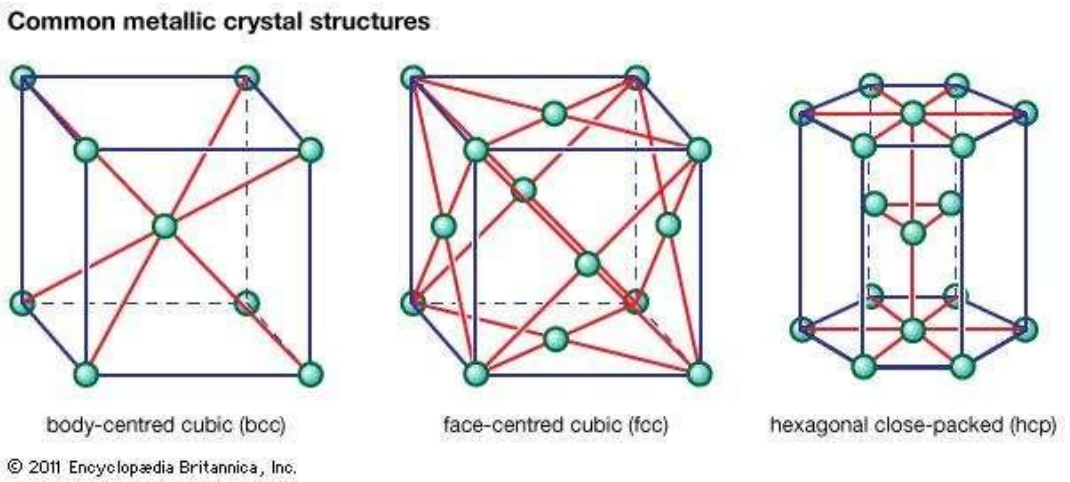
$$\hat{H}_e\left(\vec{R}_l\right) = \sum_i \frac{\hat{\vec{p}}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{\left|\vec{r}_i - \vec{r}_j\right|} - \sum_{il}\frac{Z_l e^2}{\left|\vec{r}_i - \vec{R}_l\right|}$$

Electron Hamiltonian at a given position of nuclei

Quantum Hamiltonians: General II

Adiabatic approximation: small parameter $\kappa = \left(\frac{m}{M}\right)^{1/4}$ allows to separate lattice and electron degrees of freedom

Crystals: periodic arrange of atoms

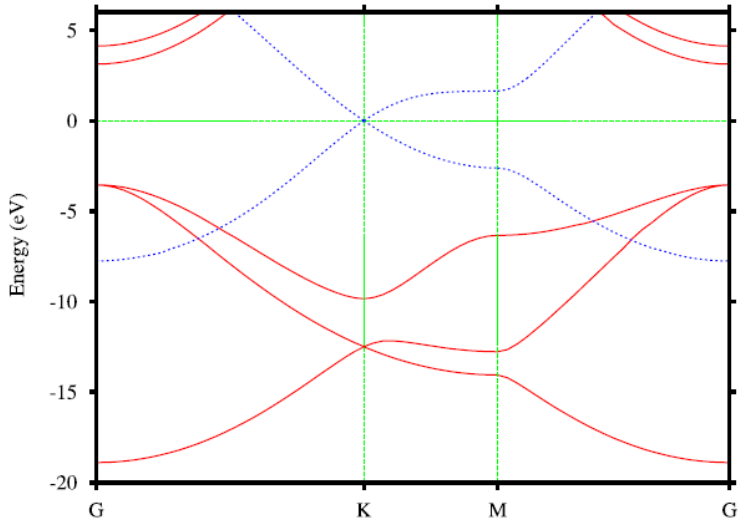


In single-electron approximation:
Bloch theorem and band structure

$$\psi_{n\vec{k}}(\vec{r}) = u_{n\vec{k}}(\vec{r})\exp\left(i\vec{k}\vec{r}\right)$$

$u_{n\vec{k}}(\vec{r})$ is periodic with the periodicity of the crystal
n is band index

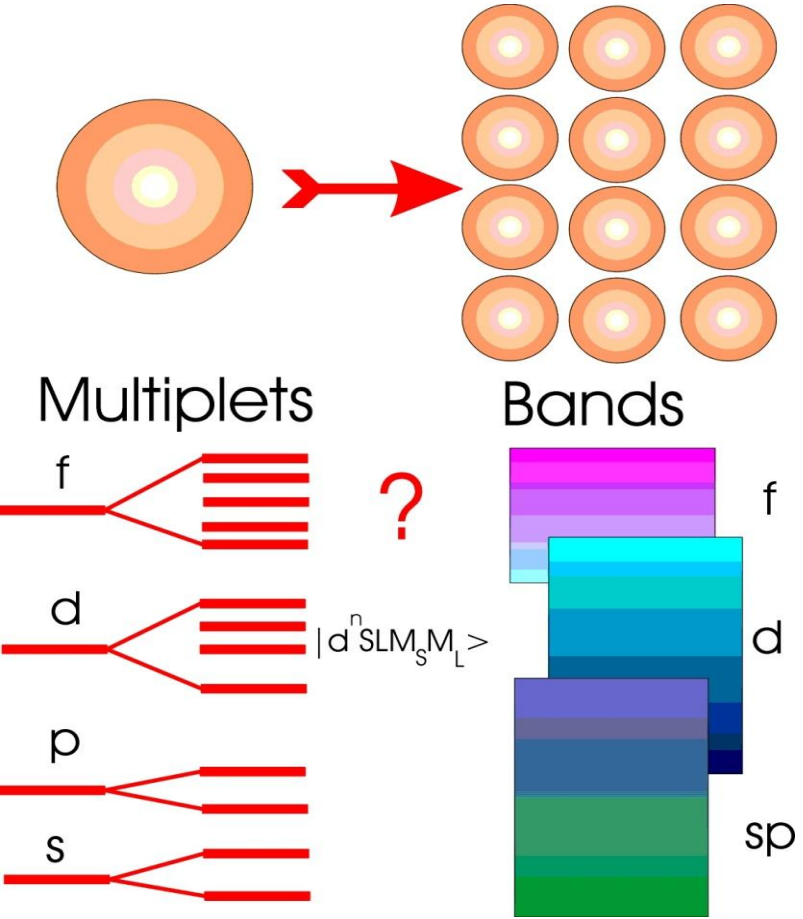
Electron energy bands in graphene



Quantum Hamiltonians: General III

The problem with this description: it neglects interelectron interaction, and the intercation is not small

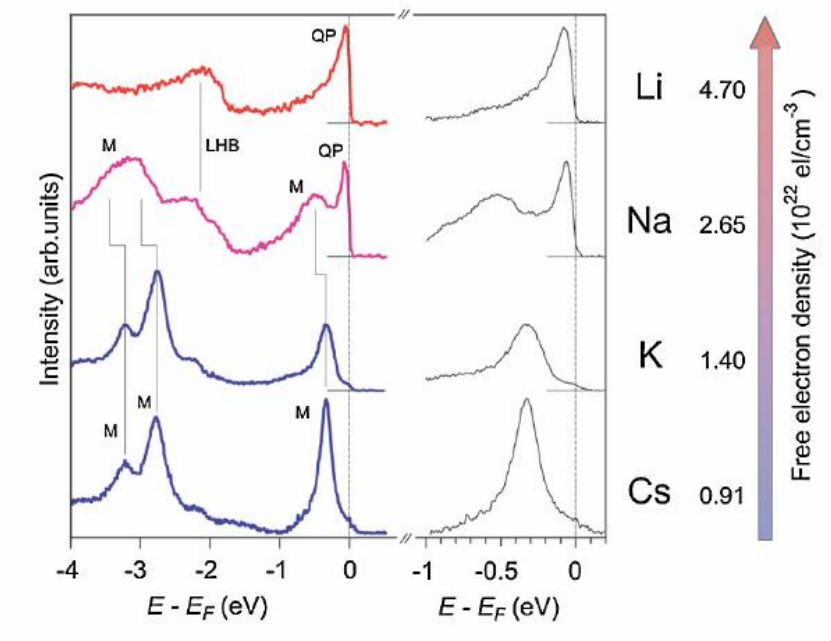
Two limits: free atoms and bands of noninteracting electrons: the description is dramatically different



PRL **104,** 117601 (2010) PHYSICAL REVIEW LETTERS week ending 19 MARCH 2010

Correlated Electrons Step by Step: Itinerant-to-Localized Transition of Fe Impurities in Free-Electron Metal Hosts

C. Carbone,[1] M. Veronese,[1] P. Moras,[1] S. Gardonio,[1] C. Grazioli,[1] P. H. Zhou,[2] O. Rader,[3] A. Varykhalov,[3] C. Krull,[4] T. Balashov,[4] A. Mugarza,[4] P. Gambardella,[4,5] S. Lebèque,[6] O. Eriksson,[7] M. I. Katsnelson,[8] and A. I. Lichtenstein[9]



Quantum Hamiltonians: General IV

To be able to do anything quantitatively we need to map initial quantum many body-problem in a crystal to an effective single-particle problem in a crystal plus auxiliary simpler many-body problem which can bve treated accurately

Auxiliary problem is homogeneous electron gas: Density Functional Theory (DFT)

Auxiliary problem is an effective atom: Dynamical Mean-Field Theory (DMFT)

Alternative approaches: GW, BSE... many words and formulas

Plus combinations

PHYSICAL REVIEW B VOLUME 57, NUMBER 12 15 MARCH 1998-I

***Ab initio* calculations of quasiparticle band structure in correlated systems: LDA++ approach**

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(Received 11 July 1997)

PHYSICAL REVIEW B VOLUME 61, NUMBER 13 1 APRIL 2000-I

First-principles calculations of magnetic interactions in correlated systems

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(Received 13 April 1999; revised manuscript received 28 October 1999)

J. Phys.: Condens. Matter **11** (1999) 1037–1048. Printed in the UK PII: S0953-8984(99)96712-7

LDA++ approach to the electronic structure of magnets: correlation effects in iron

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Received 11 August 1998

Curiosity-driven research?

Physics is like sex: sure, it may give some practical results, but that's not why we do it

R. P. Feynman

Nevertheless, we want practical results as well!

Materials for sustainability

- Optical properties (base for photonics, plasmonics, etc.);

- Magnetic properties (magnetocaloric materials, spintronics, replacement of expensive rare-earth metals on permanets magnets);

- Strength and plasticity, electronic effects on structural and thermodynamic lattice properties, phase diagrams of metals and alloys;

- Demystification of metallurgical traditional prescriptions, physics of steel;

- And much more

Optical properties of strongly correlated systems

nature communications

Article

https://doi.org/10.1038/s41467-023-41314-6

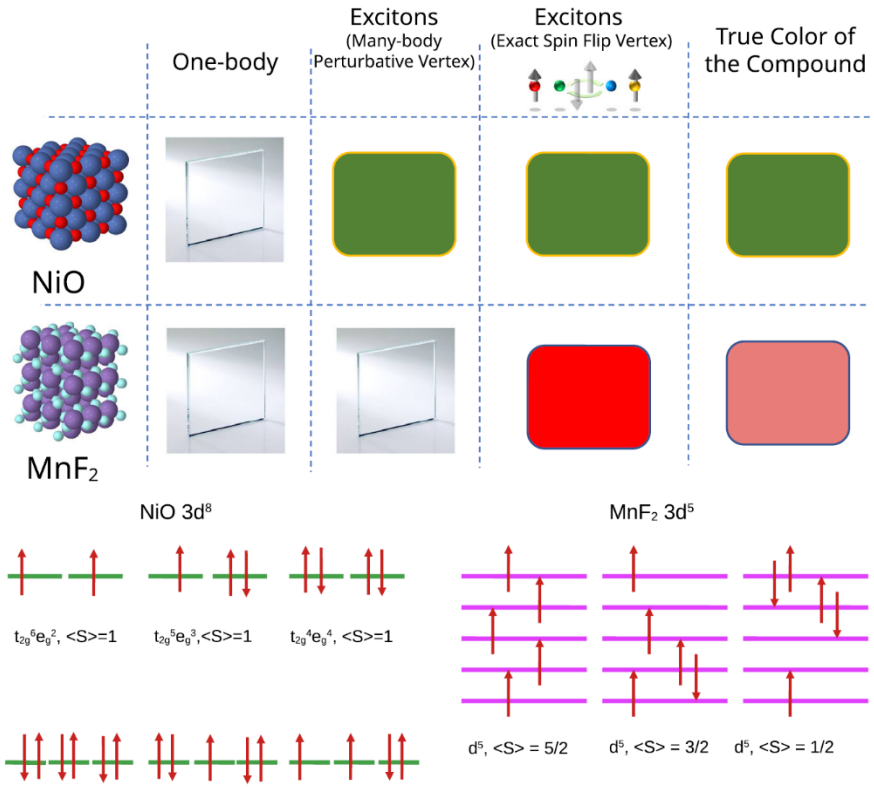
A theory for colors of strongly correlated electronic systems

Received: 4 May 2022

Accepted: 25 August 2023

Swagata Acharya[1,2], Dimitar Pashov[3], Cedric Weber[4], Mark van Schilfgaarde[2], Alexander I. Lichtenstein[5,6] & Mikhail I. Katsnelson[1]

Many strongly correlated transition metal insulators are colored, even though they have band gaps much larger than the highest energy photons from the visible light. An adequate explanation for the color requires a theoretical approach able to compute subgap excitons in periodic crystals, reliably and without free parameters—a formidable challenge. The literature often fails to disentangle two important factors: what makes excitons form and what makes them optically bright. We pick two archetypal cases as examples: NiO with green color and MnF_2 with pink color, and employ two kinds of ab initio many body Green's function theories; the first, a perturbative theory based on low-order extensions of the *GW* approximation, is able to explain the color in NiO, while the same theory is unable to explain why MnF_2 is pink. We show its color originates from higher order spin-flip transitions that modify the optical response, which is contained in dynamical mean-field theory (DMFT). We show that symmetry lowering mechanisms may determine how 'bright' these excitons are, but they are not fundamental to their existence.



Colors of very common and usual materials can be described only via subtle many-body effects and are determined by a very formal object of Feynman diagrams known as a vertex

Hyperbolic polaritons

Just to remind: crystallooptics

$$\vec{k} = k_0 \vec{n}, \qquad k_0 = \frac{\omega}{c} \qquad \det\left| n^2 \delta_{ij} - n_i n_j - \varepsilon_{ij}(\omega) \right| = 0 \qquad \varepsilon_{ij}(\omega) = \delta_{ij} + \frac{4\pi i}{\omega}\sigma_{ij}(\omega)$$

Main axes

$$\varepsilon_{ij} = \varepsilon_i \delta_{ij}$$

If $\varepsilon_x \varepsilon_y < 0$

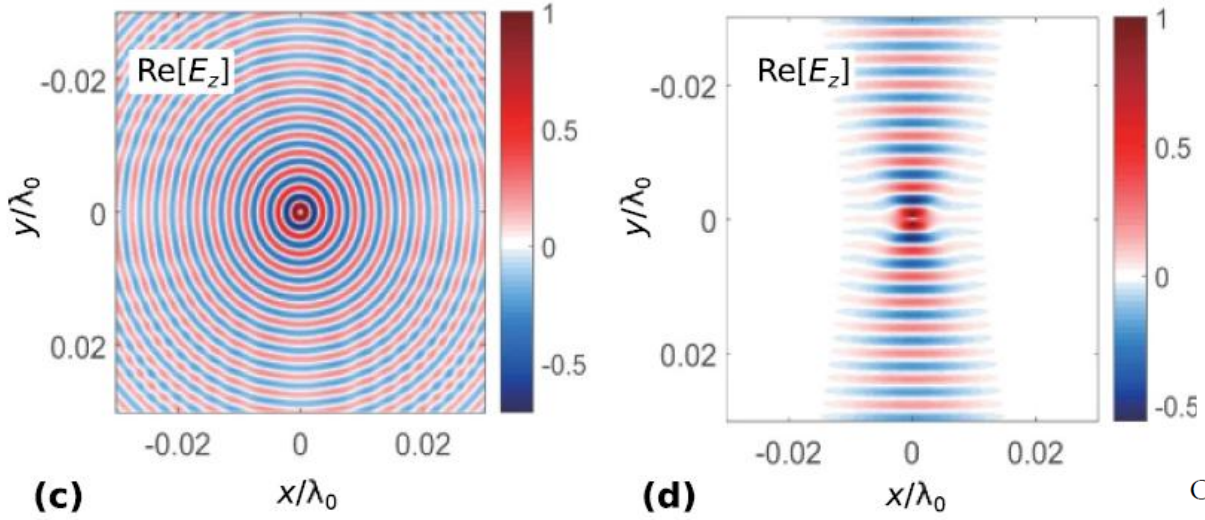
$$n_z = 0$$

$$n^2 = \varepsilon_z$$

$$\frac{n_x^2}{\varepsilon_y} + \frac{n_y^2}{\varepsilon_x} = 1$$

$$\frac{k_x^2}{|\varepsilon_y|} = \frac{k_y^2}{|\varepsilon_x|}, \qquad k >> k_0 \qquad (c \to \infty)$$

Anisotropy can result in the formation of additional types of electromagnetic waves!



Distribution of electric fields for elliptic and hyperbolic polaritons

Chang P-H, Lin C and Helmy A S 2022 Field canalization using anisotropic 2D plasmonics *npj 2D Mater. Appl.*

Hyperbolic polaritons in CrSBr

nature communications

Article

https://doi.org/10.1038/s41467-023-44100-6

Hyperbolic exciton polaritons in a van der Waals magnet

Francesco L. Ruta[1,2,12], Shuai Zhang[1,12], Yinming Shao[1,12], Samuel L. Moore[1], Swagata Acharya[3], Zhiyuan Sun[1], Siyuan Qiu[1], Johannes Geurs[1,4], Brian S. Y. Kim[1,5], Matthew Fu[1], Daniel G. Chica[6], Dimitar Pashov[7], Xiaodong Xu[8,9], Di Xiao[8,9], Milan Delor[6], X-Y. Zhu[6], Andrew J. Millis[1,10], Xavier Roy[6], James C. Hone[5], Cory R. Dean[1], Mikhail I. Katsnelson[11], Mark van Schilfgaarde[3] & D. N. Basov[1]

Experiment: observation of hyperbolic polariton at low enough temperature

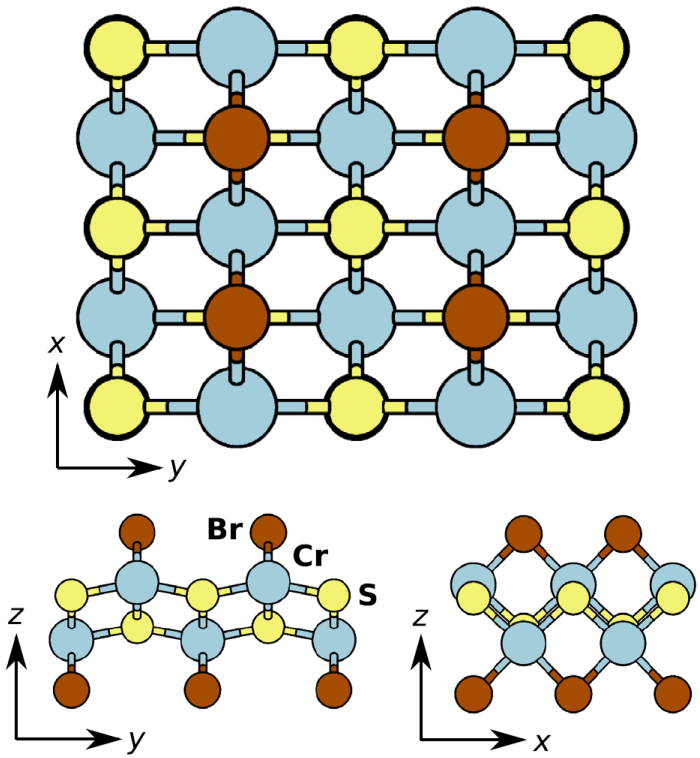
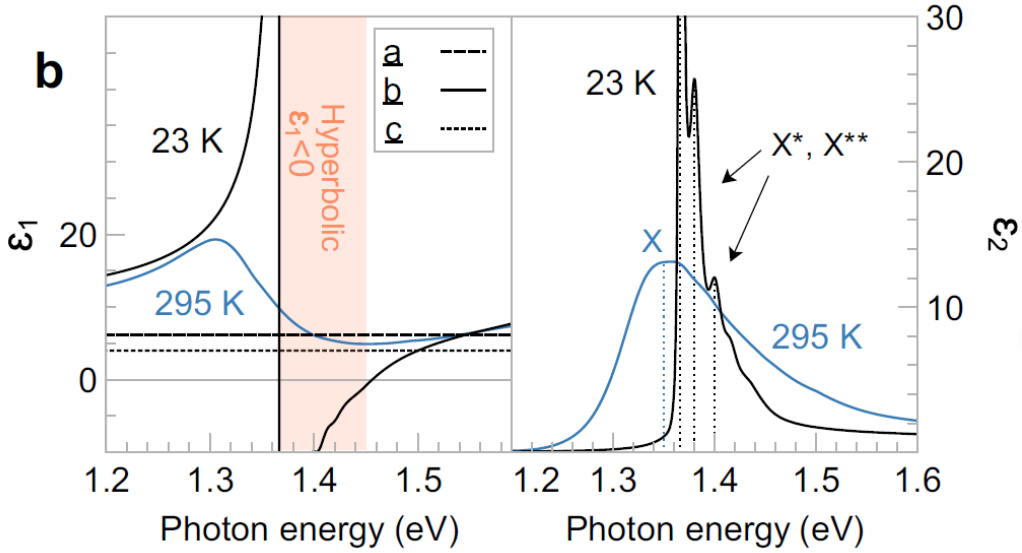


Fig. 1 Schematic crystal structure of monolayer CrSBr shown in three different projections. Brown, blue, and yellow balls correspond to Br, Cr, and S atoms, respectively.



Resonances associated to excitons (confirmed by calculations)

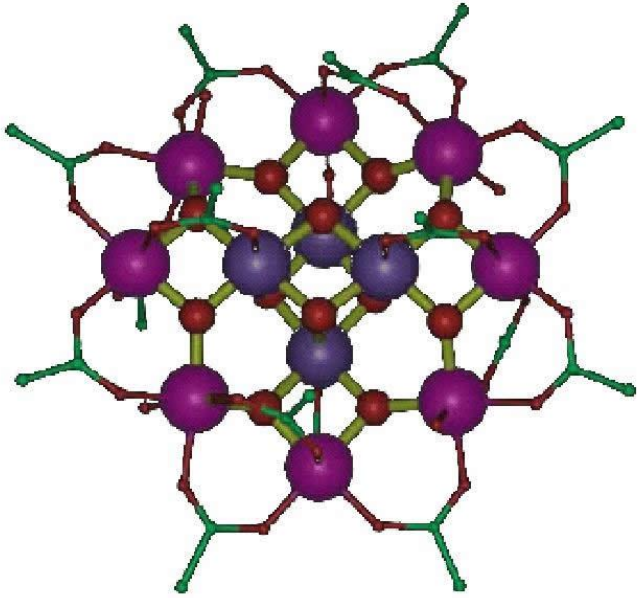
Computation of magnetic interactions

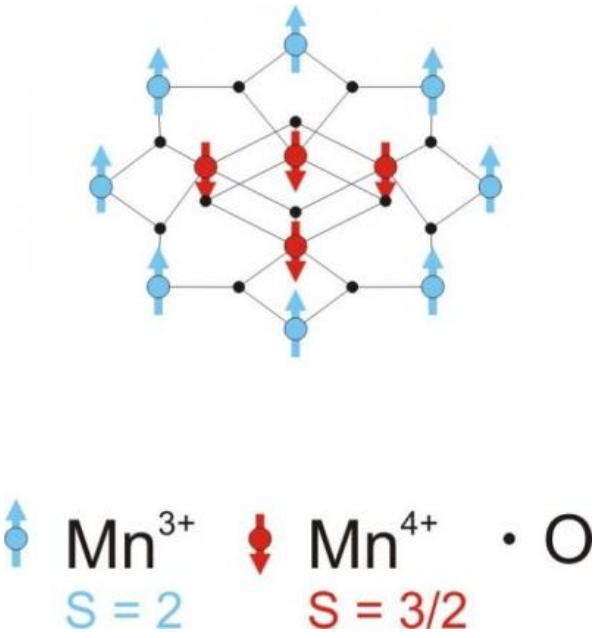
Magnetic molecules as an example of very complicated magnetic systems

PHYSICAL REVIEW B **00**, 004400 (2014)

First-principles modeling of magnetic excitations in Mn_{12}

V. V. Mazurenko,[1] Y. O. Kvashnin,[2,3] Fengping Jin,[4] H. A. De Raedt,[5] A. I. Lichtenstein,[6] and M. I. Katsnelson[1,7]





A prototype molecular magnet

Dimension of Hilbert space: $(2^{\times}2+1)^8(2^{\times}3/2+1)^4 = 10^8$

Real challenge!

$[Mn_{12}O_{12}(CH_3COO)_{16}(H_2O)_4]\cdot 2CH_3COOH\cdot 4H_2O$

Magnetic interactions in Mn12

All parameters of exchange, anisotropy and DMI calculated from first principles, after that exact diagonalization, no fitting parameters

$$\hat{H} = \sum_{ij} J_{ij} \hat{\vec{S}}_i \hat{\vec{S}}_j + \sum_{i\mu\nu} \hat{S}_i^{\mu} A_i^{\mu\nu} \hat{S}_i^{\nu} + \sum_{ij} \vec{D}_{ij} [\hat{\vec{S}}_i \times \hat{\vec{S}}_j]$$

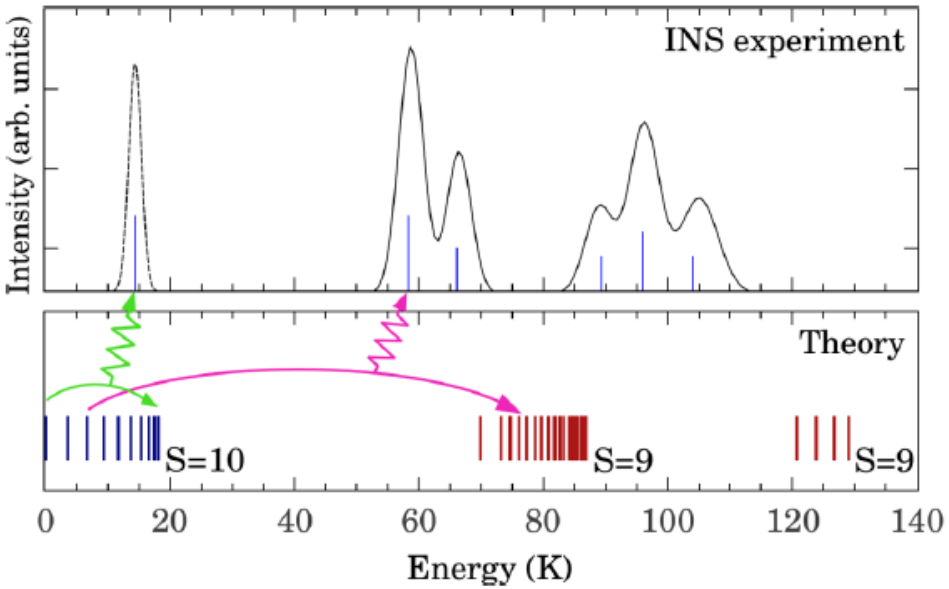
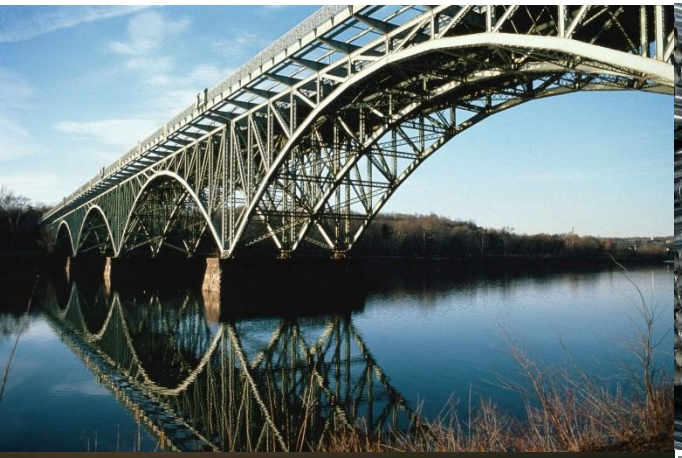


FIG. 2. (Color online) Schematic comparison of the theoretical spectrum obtained by diagonalizing Eq. (1) and INS spectrum taken from Ref. [12] (Figs. 6 and 8 therein). The arrows denote the intra- and interband transitions that correspond to the excitations observed in the INS experiment.

Also heat capacity and magnetic susceptibility have a good agreement with experiment (O. Hanebaum, J. Schnack, PRB 92, 064424 (2015))

We are still in iron age

Steel (basically, Fe and a bit C) is one of the main materials of our civilization



Physics of steel

From electronic structure to magnetism to energetics of various phases (bcc, fcc, cementite…) – then phase-field model then simulations

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]

PHYSICAL REVIEW B **90**, 094101 (2014)

Role of magnetic degrees of freedom in a scenario of phase transformations in steel

I. K. Razumov,[1,2,*] D. V. Boukhvalov,[3] M. V. Petrik,[2] V. N. Urtsev,[4] A. V. Shmakov,[4] M. I. Katsnelson,[5,6] and Yu. N. Gornostyrev[1,2]

PRL **99,** 247205 (2007) PHYSICAL REVIEW LETTERS week ending 14 DECEMBER 2007

Magnetism and Local Distortions near Carbon Impurity in γ-Iron

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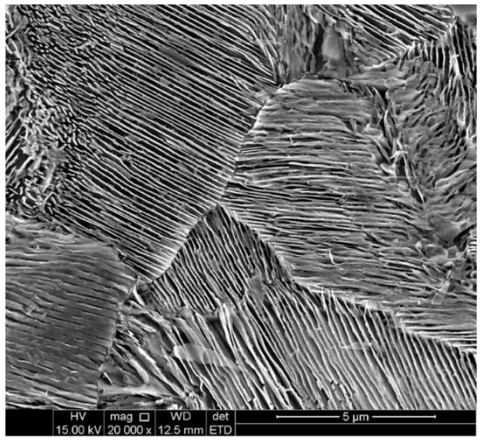
(Received 25 June 2007; published 13 December 2007)

PHYSICAL REVIEW APPLIED **7,** 014002 (2017)

Autocatalytic Mechanism of Pearlite Transformation in Steel

I. K. Razumov,[1,2,*] Yu. N. Gornostyrev,[1,2,4] and M. I. Katsnelson[3,4]

Model of pearlite structure



Pearlitic structure in rail steel (Sci Rep 9, 7454 (2019))

Long-standing problem how to explain; we made the first steps. Magnetism play a crucial role!

What to do next: (1) combine lattice and spin dynamics; (2) build better phase-field functional; (3) do three-dimensional phase-field simulations (currently we did only simplified two-dimensional model)…

A dream: the whole road from many-body quantum mechanical problem to real metallurgical processes – seems to be that all components we already have!

Collaborations in Sweden

Uppsala University (Olle Eriksson group)
KTH (Anna Delin group)
Linköping University (Igor Abrikosov group)

Clear opportunities to establish collaboration with Lund (including MAX IV Lab and ESS) and Lulea (steel!)

MANY THANKS FOR YOUR ATTENTION