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Theory of Graphene at IMM: Creating a Language for the New World

Mikhail Katsnelson

20th jubilee edition of the IMM Symposium, November 2026

Pre-history: the group before IMM



Aloysio Janner (1928-2016)

Main subject: multidimensional crystallography (turned out to be important after discovery of quasicrystals which are 3-dim projection of 6-dim crystals)



Ted Janssen (1936-2017)



The tenth Ewald Prize has been awarded to Professors A. Janner and T.W.J.M. Janssen (both from the Institute for Theoretical Physics, University of Nijmegen, The Netherlands) for the development of superspace crystallography and its application to the analysis of aperiodic crystals.

Pre-history: carbon for the group and for me



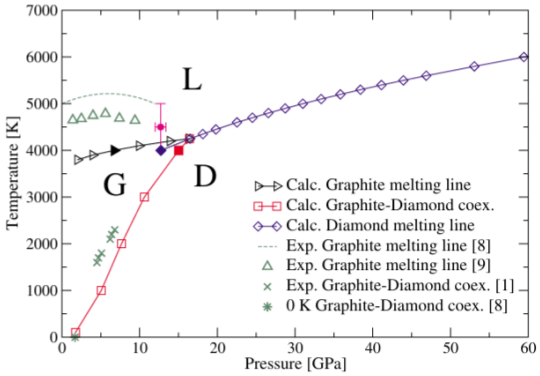
Annalisa Fasolino

Novel potential for carbon

PHYSICAL REVIEW B **68**, 024107 (2003)

Intrinsic long-range bond-order potential for carbon: Performance in Monte Carlo simulations of graphitization

J. H. Los and A. Fasolino
Theoretical Physics, NSRIM, University of Nijmegen, Toernooiveld, 6525 ED Nijmegen, The Netherlands
(Received 11 February 2003; published 31 July 2003)





Jan Los

PRL **94,** 145701 (2005) PHYSICAL REVIEW LETTERS week ending 15 APRIL 2005

Modeling the Phase Diagram of Carbon

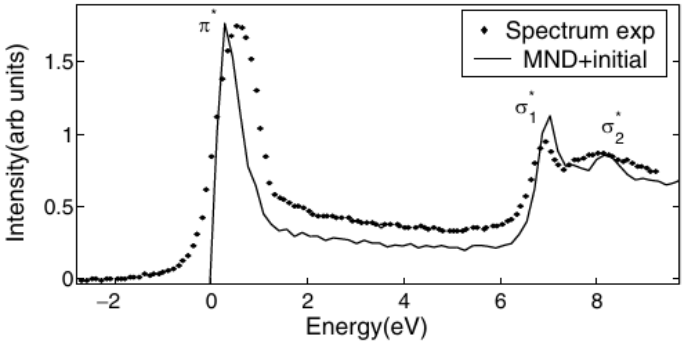
Luca M. Ghiringhelli,[1] Jan H. Los,[2] Evert Jan Meijer,[1] A. Fasolino,[1,2] and Daan Frenkel[1,3]
[1]*van 't Hoff Institute for Molecular Sciences, Universiteit van Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands*
[2]*Theoretical Physics, IMM, Radboud University Nijmegen, Toernooiveld, 6525 ED Nijmegen, The Netherlands*
[3]*FOM Institute for Atomic and Molecular Physics, Kruislaan 407, 1098 SJ, Amsterdam, The Netherlands*
(Received 9 December 2004; published 13 April 2005)

Meanwhile in Uppsala…

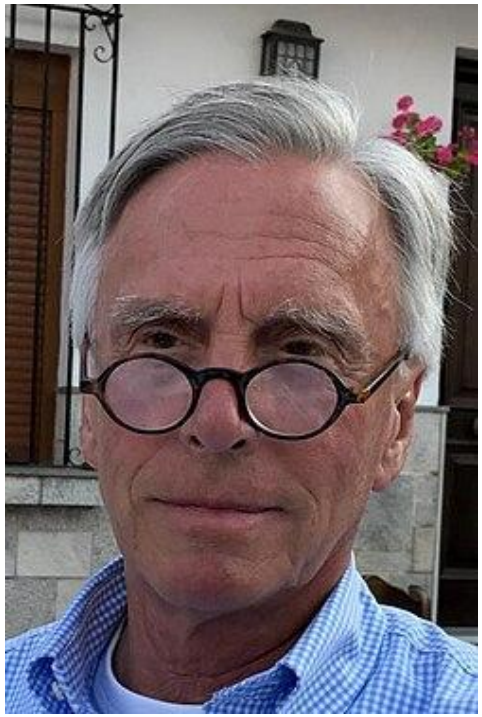
PRL **94,** 167401 (2005) PHYSICAL REVIEW LETTERS week ending 29 APRIL 2005

***Ab Initio* Theory of Dynamical Core-Hole Screening in Graphite from X-Ray Absorption Spectra**

O. Wessely,[1] M. I. Katsnelson,[1,2] and O. Eriksson[1]
[1]*Department of Physics, Uppsala University, Box 530, SE-75121, Uppsala, Sweden*
[2]*Institute for Molecules and Materials, Radboud University, NL-6525 ED Nijmegen, The Netherlands*
(Received 20 September 2004; published 26 April 2005)



Beginning: soft matter and chemistry



Roeland Nolte (1944-2024)

After discussing with Roeland I decided: let us do some soft matter

And we did!

30

THE JOURNAL OF PHYSICAL CHEMISTRY B LETTERS

2006, *110,* 30−32

Published on Web 12/10/2005

Solvent-Driven Formation of Bolaamphiphilic Vesicles

M. I. Katsnelson and A. Fasolino*

Institute for Molecules and Materials, Radboud University Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands

Received: October 11, 2005; In Final Form: November 29, 2005

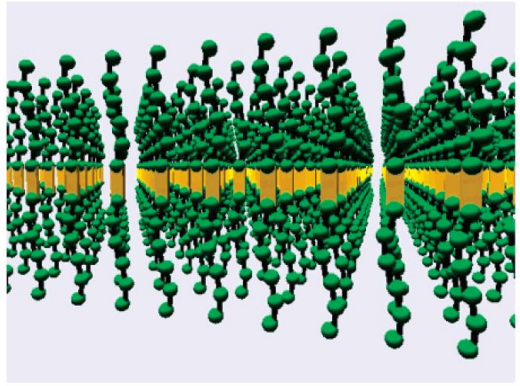


Figure 2. Sketch of a layer formed by self-assembled bolaamphiphiles. The spacing between hydrophilic tails (green) is fixed by the hydrophobic cores (yellow) to a value which might be not optimal for tail–solvent interactions.

$$\mathcal{F}_{\text{el}} = \int dS[A'K + AH^2 + c_1H^4 + c_2H^2K + c_3K^2]$$

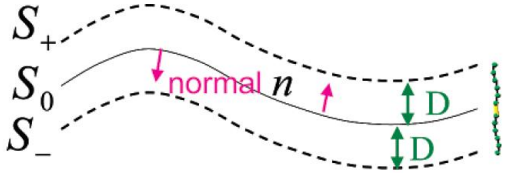
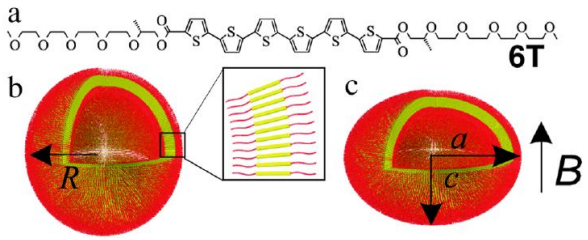


Figure 3. Schematic geometry of our model. The surface S_0 is the locus of the center of mass of the hydrophobic cores and $S_\pm$ are the surfaces formed by the tail ends. The unit vector $\vec{n}$ is normal to all three surfaces and D is the effective tail length.

PRL **98,** 146101 (2007) PHYSICAL REVIEW LETTERS week ending 6 APRIL 2007

Anharmonic Magnetic Deformation of Self-Assembled Molecular Nanocapsules

O. V. Manyuhina,[1] I. O. Shklyarevskiy,[1,2] P. Jonkheijm,[2] P. C. M. Christianen,[1,*] A. Fasolino,[1] M. I. Katsnelson,[1] A. P. H. J. Schenning,[2] E. W. Meijer,[2] O. Henze,[3] A. F. M. Kilbinger,[3] W. J. Feast,[2,3] and J. C. Maan[1]



…And then Roeland said: yeah, but spherical vesicles are not very typical and not very important. Can you do fibers?

What about graphene?

October/November 2004; PhD defense of Kostya Novoselov (supervisors Jan Kees Maan and Andre Geim); subject: magnetism

Me: Let us discuss magnetic Peierls relief.

AG: Who cares on magnetism? What about massless Dirac fermions in magnetic field?

Me: (refered to Atiyah-Singer theorem)

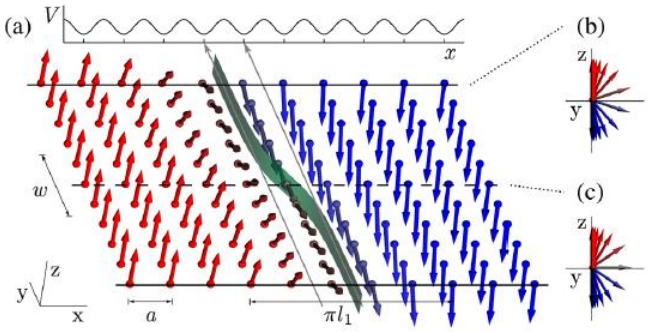
AG: (impressed)

But, after 10 years:

PRL 113, 217202 (2014) PHYSICAL REVIEW LETTERS week ending 21 NOVEMBER 2014

Motion of Domain Walls and the Dynamics of Kinks in the Magnetic Peierls Potential

F. J. Buijnsters,* A. Fasolino, and M. I. Katsnelson
Institute for Molecules and Materials, Radboud University Nijmegen, Heyendaalseweg 135, 6525 AJ Nijmegen, Netherlands
(Received 25 July 2014; published 17 November 2014)



Motivation:

Subatomic movements of a domain wall in the Peierls potential

K. S. Novoselov[1], A. K. Geim[1], S. V. Dubonos[3], E. W. Hill[2] & I. V. Grigorieva[1]

NATURE | VOL 426 | 18/25 DECEMBER 2003

Discovery of massless Dirac fermions

Vol 438|10 November 2005|doi:10.1038/nature04233 nature

LETTERS

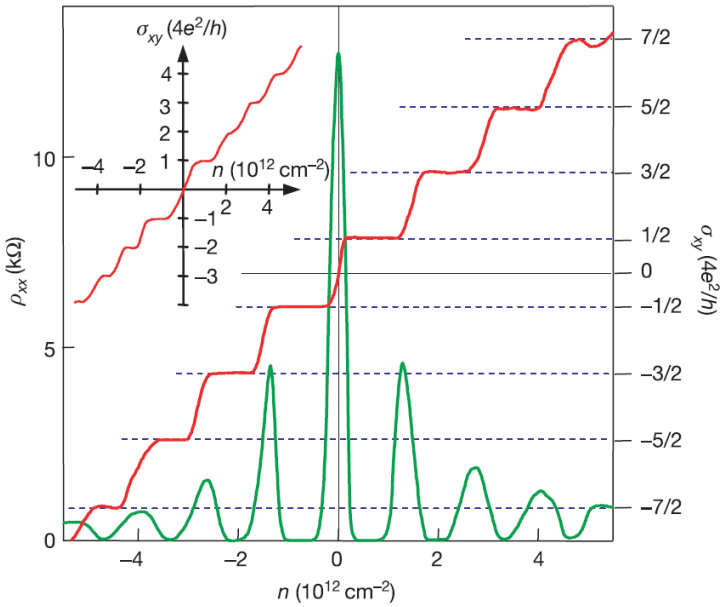
Two-dimensional gas of massless Dirac fermions in graphene

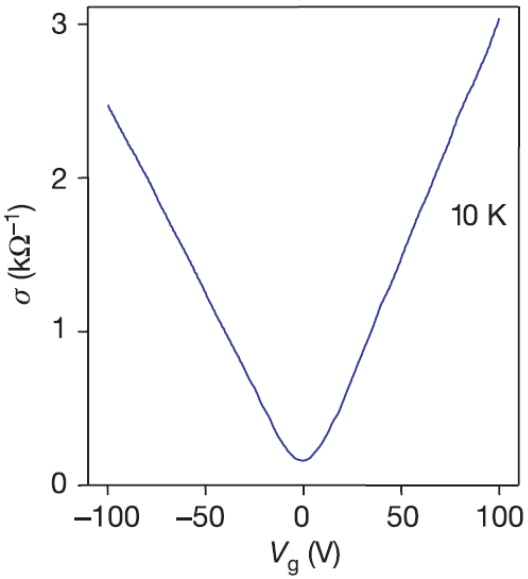
K. S. Novoselov[1], A. K. Geim[1], S. V. Morozov[2], D. Jiang[1], M. I. Katsnelson[3], I. V. Grigorieva[1], S. V. Dubonos[2] & A. A. Firsov[2]

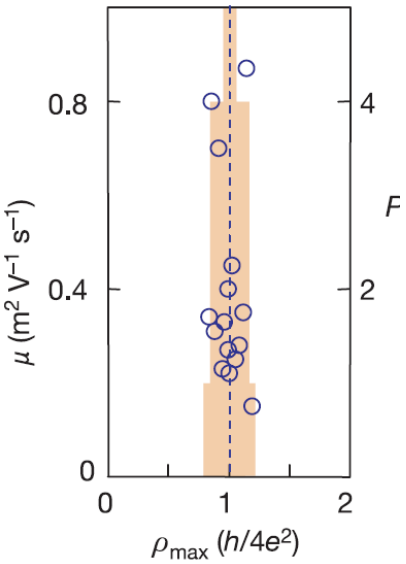
Two most mysterious observations:

(1) Half-integer quantum Hall effect;

(2) Minimal conductivity







Discovery of massless Dirac fermions

Graphene: carbon in two dimensions

Mikhail I. Katsnelson
Institute for Molecules and Materials, Radboud University Nijmegen, 6525 ED Nijmegen, The Netherlands

20 materialstoday JAN-FEB 2007 | VOLUME 10 | NUMBER 1-2

Index theorem

The deepest view on the origin of the zero-energy Landau level, and thus the anomalous QHE is provided by an Atiyah-Singer index, theorem that plays an important role in modern quantum field

Eur. Phys. J. B **51**, 157–160 (2006)
DOI: 10.1140/epjb/e2006-00203-1

THE EUROPEAN PHYSICAL JOURNAL B

Zitterbewegung, chirality, and minimal conductivity in graphene

M.I. Katsnelson[a]

Institute for Molecules and Materials, Radboud University Nijmegen, 6525 ED Nijmegen, The Netherlands

Received 6 May 2006
Published online 30 May 2006 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2006

The result $\sigma = e^2/(\pi h)$ per valley per spin is found here for the case of ideal crystal.

"Missing pi(e) problem"; in better samples theory turns out to be close to experiment

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

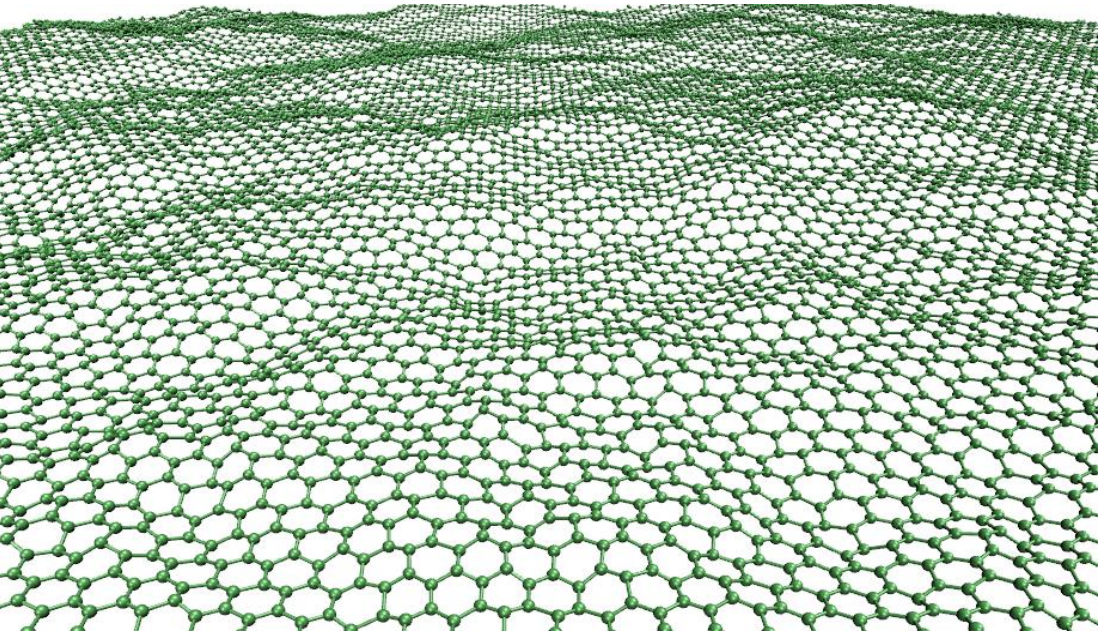
Yang Wang,[1,2]* Dillon Wong,[1,2]* Andrey V. Shytov,[3] Victor W. Brar,[1,2] Sangkook Choi,[1] Qiong Wu,[1,2] Hsin-Zon Tsai,[1] William Regan,[1,2] Alex Zettl,[1,2] Roland K. Kawakami,[5] Steven G. Louie,[1,2] Leonid S. Levitov,[4] Michael F. Crommie[1,2]†

10 MAY 2013 VOL 340 SCIENCE

Atomistic simulations, ripples and all that

Suspended graphene is (intrinsically) rippled, in agreement with experiment

Fasolino, Los, Katsnelson, Nat. Mater. 2007,
Los, Katsnelson,Yazyev, Zakharchenko, Fasolino PRB (RC) 2009



Monte-Carlo snapshot at room temperature

ripples appear, no topological defects, fixed connectivity

broad distribution of ripple sizes

Atomistic simulations, ripples and all that II

PHYSICAL REVIEW B **106**, 045418 (2022)

Distribution of ripples in graphene membranes

Jin Yu,[1,2,3] Mikhail I. Katsnelson,[2] Tianzhong Zhang,[1] and Shengjun Yuan[4,2]

Intrinsic ripples with various configurations and sizes were reported to affect the physical and chemical properties of two-dimensional (2D) materials. By performing molecular dynamics simulations and theoretical analysis, we use two geometric models of the ripple shape to explore numerically the distribution of ripples in the graphene membrane. We focus on the ratio of the ripple height to its diameter (t/D) which was recently shown to be the most relevant for chemical activity of graphene membranes. Our result demonstrates that the ripple density decreases as the coefficient t/D increases, in qualitative agreement with the Boltzmann distribution derived analytically from the bending energy of the membrane. Our theoretical paper provides also specific quantitative information on the ripple distribution in graphene and gives new insights applicable to other 2D materials.

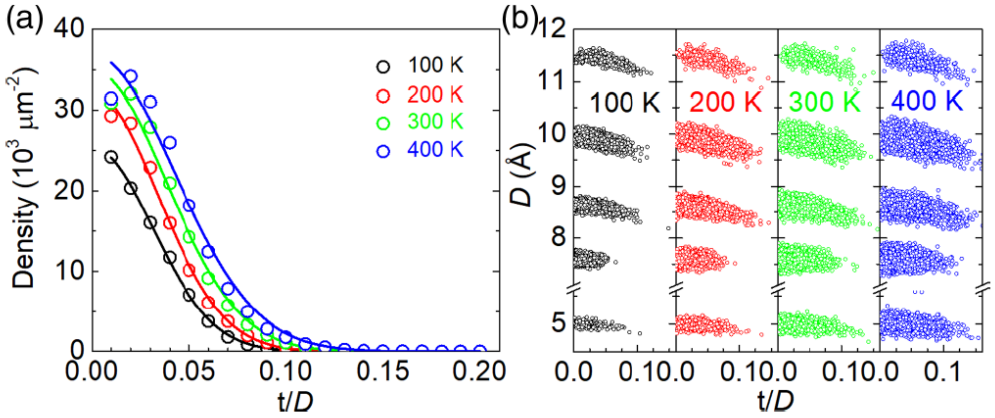


FIG. 2. (a) Ripple density and (b) size D as a function of t/D in graphene membrane with the circlelike model. The circles are statistical data from MD simulations and the solid lines are fit results using Eq. (2). Black, red, green, and blue represent for 100, 200, 300, and 400 K, respectively.

Ripples and all that III

One of the main directions of group activity for decades, from simulations to quantum-field-style theories

ACCOUNTS of chemical research

Graphene as a Prototype Crystalline Membrane

MIKHAIL I. KATSNELSON* AND ANNALISA FASOLINO
Institute for Molecules and Materials, Radboud University Nijmegen, Heyendaalseweg 135, 6525AJ Nijmegen, The Netherlands

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER
J. Phys.: Condens. Matter **23** (2011) 202202 (4pp) doi:10.1088/0953-8984/23/20/202202

FAST TRACK COMMUNICATION

Melting of graphene: from two to one dimension

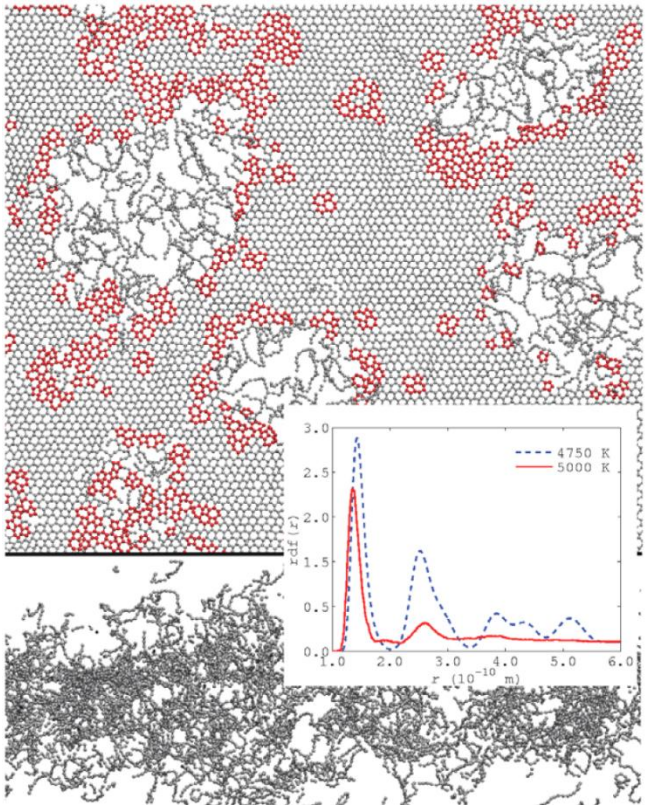
K V Zakharchenko, Annalisa Fasolino, J H Los and M I Katsnelson

npj | 2D Materials and Applications

ARTICLE **OPEN**

Mechanics of thermally fluctuating membranes

J. H. Los[1], A. Fasolino[1] and M. I. Katsnelson[1]



Ripples and all that IV

Available online at www.sciencedirect.com
ScienceDirect
Nuclear Physics B 956 (2020) 115040
www.elsevier.com/locate/nuclphysb

Scaling behavior of crystalline membranes: An ε-expansion approach

Achille Mauri *, Mikhail I. Katsnelson

Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, the Netherlands

Available online at www.sciencedirect.com
ScienceDirect
Nuclear Physics B 969 (2021) 115482
www.elsevier.com/locate/nuclphysb

Scale without conformal invariance in membrane theory

Achille Mauri *, Mikhail I. Katsnelson

Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, the Netherlands

PHYSICAL REVIEW B **105**, 195434 (2022)

Editors' Suggestion

Perturbative renormalization and thermodynamics of quantum crystalline membranes

Achille Mauri * and Mikhail I. Katsnelson

Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands

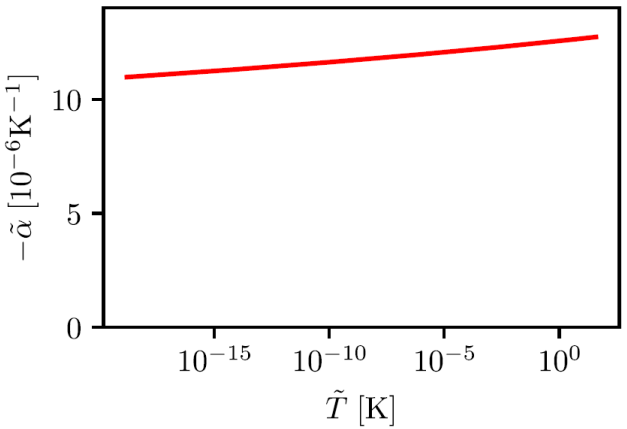


FIG. 3. Negative thermal expansion coefficient for an unstressed graphene membrane as a function of temperature (red solid line). In the limit $T \to 0, \tilde{\alpha} \to 0$ as expected from the third law of thermodynamics, but the approach to zero is only logarithmic with $\tilde{T}$.

And many other things

- Chemistry of graphene (including participation in discovery of graphene and fluorographene, anomalous penetration of hydrogen through graphene, role of ripples in chemical activity of graphene)
- Mechanisms of electronic transport in graphene (role of resonant impurities, ripples, clusters of charge impurities, two-phonon processes etc.)
- Structure of twisted bilayer graphene and graphene at hBN
- Graphene tunneling transistor and graphene single-electron transistor
- Last not list: development of general language in graphene science

Physics Reports 496 (2010) 109–148

Contents lists available at ScienceDirect

Physics Reports

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

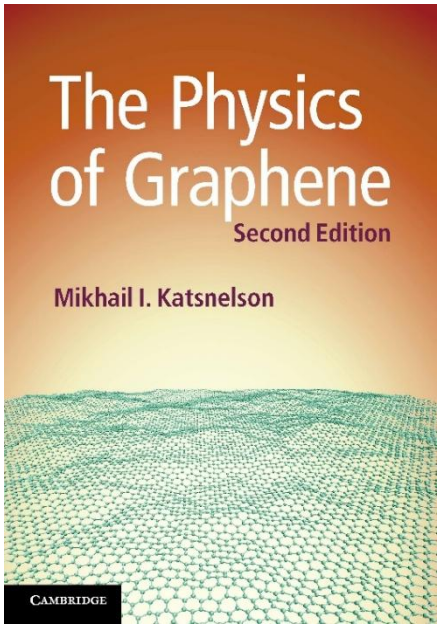


Gauge fields in graphene

M.A.H. Vozmediano [a], M.I. Katsnelson [b], F. Guinea [a,*]

[a] Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, E-28049 Madrid, Spain

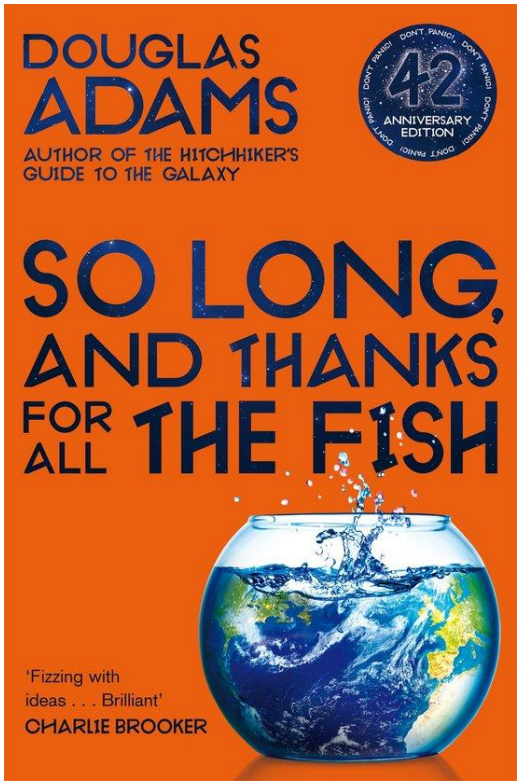
[b] Radboud University Nijmegen, Institute for Molecules and Materials, Heijendaalseweg 135, 6525 AJ, Nijmegen, The Netherlands



To conclude

- We did many other things apart from graphene (magnetism, strongly correlated systems, quantum transport, physics of complexity, even foundations of quantum mechanics)
- It was really great to do theoretical condensed matter physics within IMM
- Let us hope it will be the same (or even better) in the future

So long, and thanks for all the fish



AND MANY THANKS FOR YOUR ATTENTION