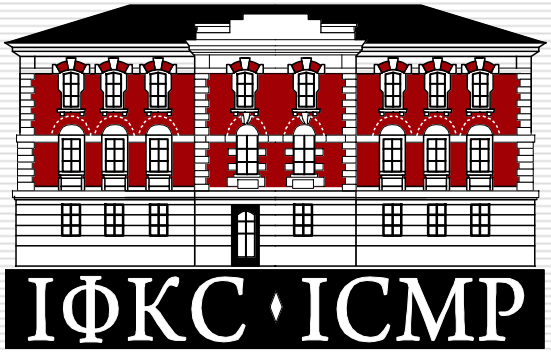
Leopolis Scientica

Scientific heritage versus modern trends in statistical physics



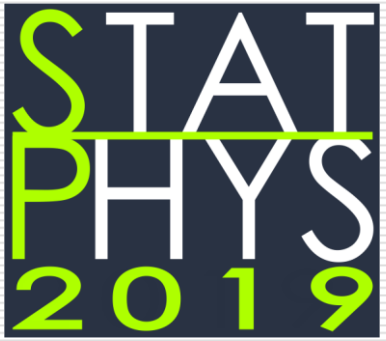
Andrij Trokhymchuk
Institiute for Condensed Matter Physics
Natl Acad Sci of Ukraine

@

5-th meeting on Statistical Physics:

July 3-6, 2019

Lviv



Leopolis Scientifica: Scientific heritage versus modern trends in statistical physics

Andrij Trokhymchuk

Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv 79011, Ukraine E–mail: adt@icmp.lviv.ua

Scientific heritage of Lviv is rather diverse including names, schools, traditions, buildings, and museums associated with various fields of science such as philosophy, astronomy, physics, mathematics, medicine, chemistry, biology, etc.

Keeping in mind the primary topics of Statphys 2019, namely: (i) modern trends and applications in statistical physics and (ii) the 110th anniversary of M M Bogolyubov, main attention of this contribution will be turned out to the names of Marian Smoluchowski and Department for Theoretical Physics of Lviv University, Stanislav Ulam and Lviv Polytechnic University, Stefan Banach and Lviv school of mathematics, as well as Igor Yukhnovskii and Institute for Condensed Matter Physics.

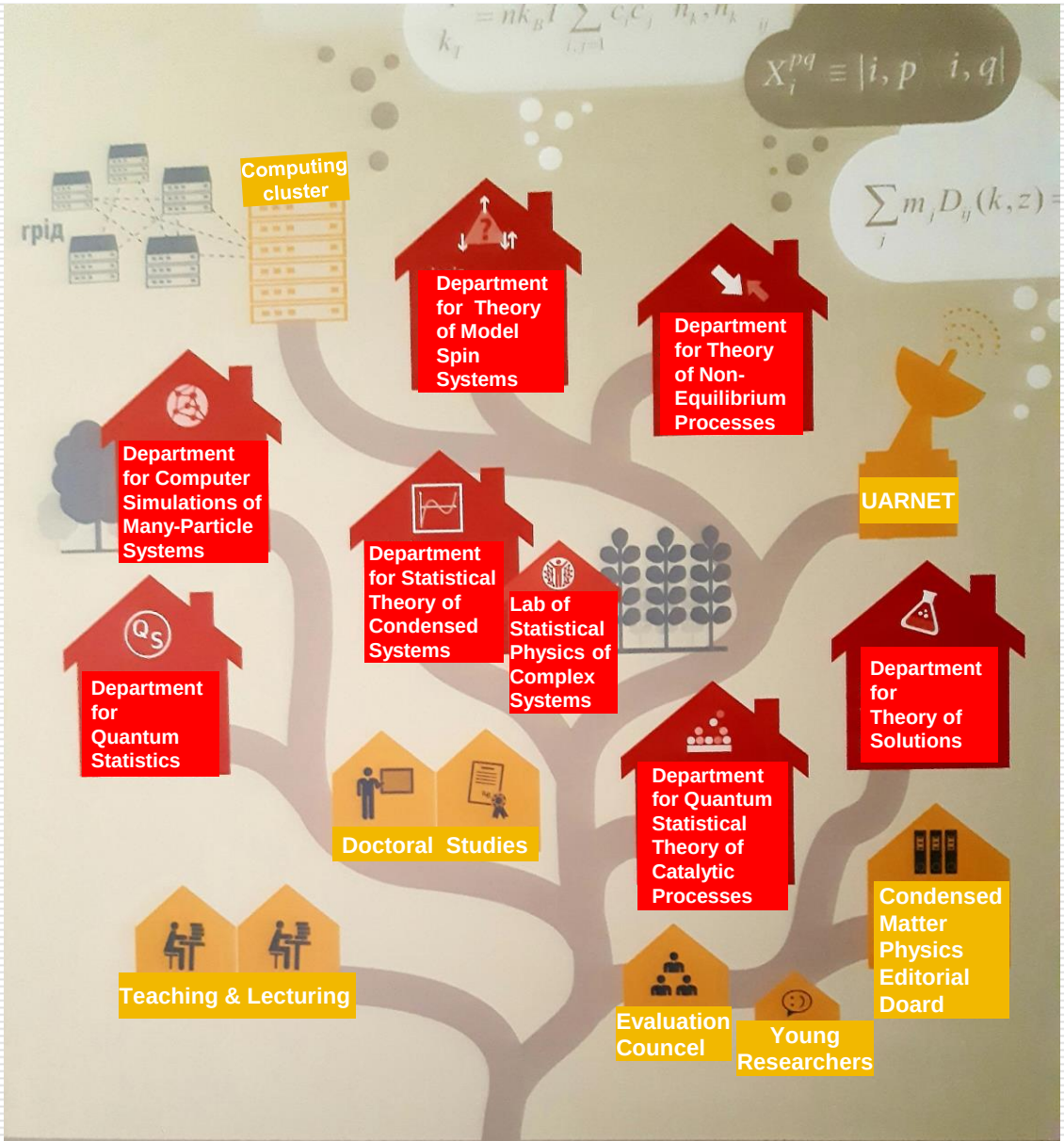
Institute for Condensed Matter Physics of the Natl. Acad. Sci. of Ukraine

1969 Lviv **Department for Statistical Theory of Condensed Matter** @ Institute for Theoretical Physics (Kyiv) of the Academy of Sciences of Ukr SSR

1980 Lviv **Division of Statistical Physics** @ Institute for Theoretical Physics (Kyiv) of the Academy of Sciences of Ukr SSR, composed of 3 Departments:
Department for Statistical Theory of Condensed Matter,
Department for Theory of Solutions,
Department for Quantum Statistics

1990 **Institute for Condensed Matter Physics** of the Academy of Sciences of Ukr SSR

Institute for Condensed Matter Physics of the Natl. Acad. Sci. of Ukraine as of 2003




Europe
International Boundary
Road
River
National Capital
City or Town
0 250 500 KM
0 250 500 Miles
© 2007 Geology.com
Reykjavik
Thjorsa
ICELAND
Norwegian Sea
Barents Sea
Faroe Islands
Shetland Islands
SWEDEN
FINLAND
NORWAY
RUSSIA
Trondheim
Osterdalalven
Gulf of Bothnia
Lake Onega
Lake Ladoga
Pechora
Ob'
Irtysh
Vychegda
Kama
Sukhona
Tobol
Perm'
Yekaterinburg
Chelyabinsk
Ufa
Bergen
Oslo
Turku
Helsinki
St. Petersburg
Kostroma
Kazan'
Yaroslavl'
Ural
Nizhniy Novgorod
Volga
Stockholm
Tallinn
ESTONIA
U.K.
Glasgow
Edinburgh
Belfast
IRELAND
Dublin
Cork
Liverpool
Manchester
Birmingham
Bristol
London
Goteborg
DENMARK
North Sea
Arhus
Copenhagen
Malmo
Baltic Sea
Liepaja
Riga
LATVIA
Daugavpils
LITHUANIA
Vilnius
Minsk
Moscow
Ryazan'
Tula
KAZAKHSTAN
Atlantic Ocean
NETHERLANDS
Amsterdam
BELGIUM
Antwerp
Brussels
Gdansk
RUSSIA
BELARUS
Voronezh
Berlin
Warsaw
POLAND
Lodz
GERMANY
UZBEKISTAN
Kiev
Kharkiv
Don
Paris
Prague
CZECH REP.
Krakow
UKRAINE
Donets'k
Volga
LUXEMBOURG
Nantes
SWITZERLAND
LIECHTENSTEIN
L'viv
Dnipropetrovs'k
Rostov
Bay of Biscay
FRANCE
Bern
Vienna
Bratislava
SLOVAKIA
MOLDOVA
Caspian Sea
AUSTRIA
Budapest
Chisinau
Lyon
HUNGARY
Odesa
Gijon
Milan
SLOVENIA
Ljubljana
ROMANIA
TURKMENISTAN
Bilbao
Turin
Zagreb
Brasov
Oporto
Valladolid
Toulouse
CROATIA
Genoa
SAN MARINO
BOSNIA & HERZE.
Belgrade
GEORGIA
Tiflis
Baku
Duero
Zaragoza
Marseille
Florence
SERBIA
Bucharest
Black Sea
ARMENIA
PORTUGAL
ANDORRA
MONACO
Sarajevo
AZERBAIJAN
Lisbon
Madrid
ITALY
MONTENEGRO
BULGARIA
Yerevan
Barcelona
Corsica
Podgorica
Sofia
Guadiana
Rome
Skopje
Istanbul
Tabriz
SPAIN
Sevilla
Valencia
Tirana
MACEDONIA
Naples
Bari
ALBANIA
Ankara
Murat
IRAN
Tehran
Thessaloniki
Malaga
Murcia
Sardinia
Cagliari
Bursa
TURKEY
Tigris
Qom
GIBRALTAR
Mediterranean Sea
GREECE
Mosul
Palermo
Izmir
Casablanca
Rabat
Algiers
Athens
Adana
Kermanshah
Aleppo
Euphrates
Constantine
Tunis
Catania
Sicily
SYRIA
Baghdad
Nicosia
Ahvaz
CYPRUS
MOROCCO
MALTA
Mediterranean Sea
Crete
Beirut
Damascus
IRAQ
Basra
LEBANON
TUNISIA
Tripoli
ALGERIA
'Amman
Kuwait
ISRAEL
Jerusalem
KUWAIT
WESTERN SAHARA
JORDAN
Alexandria
SAUDI ARABIA
LIBYA
Cairo
MAURITANIA
EGYPT
L

1245 - 1349

King of Galicia and Volhynia (King of Rus')

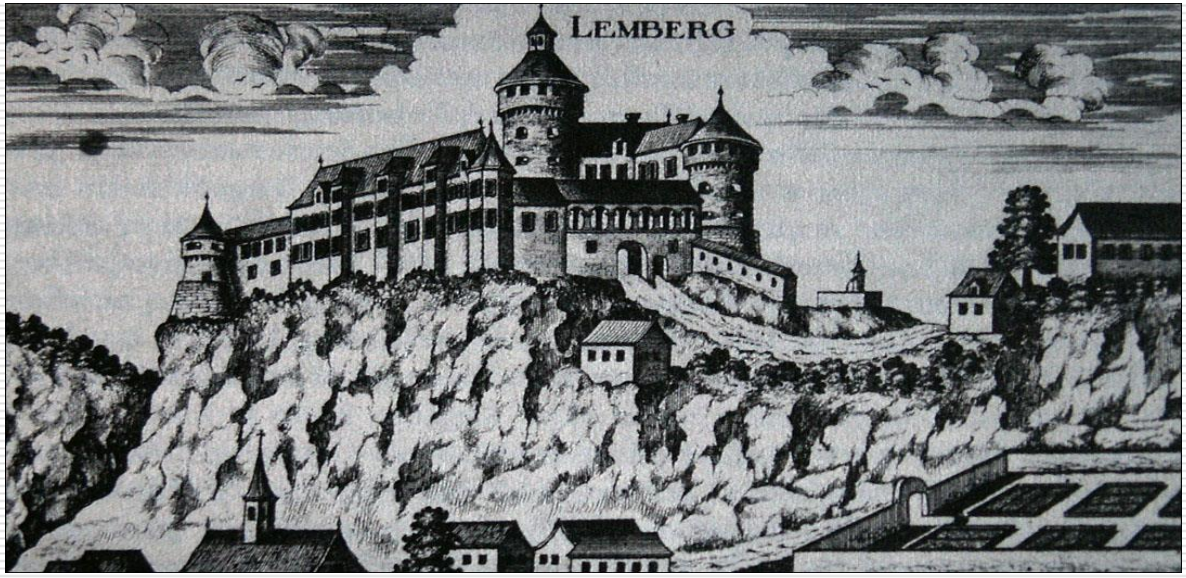
Reign	1253–1264
Predecessor	title created
Successor	Lev Danylovych

Grand Prince of Kiev

Reign	1240–1264
Predecessor	Roman the Great
Successor	Lev I of Galicia

Born	1201 Halych (now Ukraine)
Died	1264 Kholm (modern Chełm, Poland)

Lviv/Leopolis/Lemberg/Lwow
1256



King Lev

King Danylo

Polish-Lithuanian Commonwealth 1635

1804 - 1918

Austrian Empire Provinces

German Empire

Russian Empire

Bohemia

Silesia

Galicia

Lemberg (Lviv)

Moravia

Upper Austria

Lower Austria

Hungary

Bukovina

Vorarlberg

Salzburg

Styria

Tirol

Carinthia

Hungarian Empire

Carniola

Croatia and Slavonia

Kustenland

Bosnia and Herzegovina

Italy

Dalmatia

Ottoman Empire

Adriatic

1920 - 1939


Telšiai
Šiauliai
Daugavpils
Memel
Polotsk
Kėdainiai
Kaunas
Święciany
Wilno
Königsberg
Gdynia
Danzig
Stolp
Alytus
Oszmiana
Wilejka
Sejny
Suwałki
Marienburg
Lyck
Allenstein
Grodno
Lida
Minsk
Borisov
Schneidemühl
Bydgoszcz
Grudziądz
Toruń
Mława
Łomża
Mosty
Nowogródek
Wołkowysk
Białystok
Baranowicze
Slutsk
Inowrocław
Poznań
Płock
Modlin
Warszawa
Siedlce
Brześć
Pińsk
Mikaszewicze
Mozyr
Leszno
Łódź
Ostrów Wlkp.
Glogau
Breslau
Dęblin
Maniewicze
Kowel
Sarny
Chełm
Lublin
Częstochowa
Kielce
Włodzimierz
Oppeln
Sandomierz
Zamość
Łuck
Równe
Zviahel
Zhytomir
Sosnowiec
Katowice
Kraków
Tarnów
Brody
Ostrava
Olomouc
Przemyśl
Lwów
Berdychov
Cieszyn
Nowy Targ
Nowy Sącz
Tarnopol
Brno
Žilina
Stryj
Vinnitsa
Trenčín
Prešov
Stanisławów
Banská Bystrica
Košice
Kamyanets Podolskiy
Bratislava
Nitra
Cernăuți
Poland
USSR

1944 - 1991


Ukraine
Moscow
SOVIET UNION
L
U S S R
Republic boundary
Autonomous republic (ASSR) or oblast boundary
Republic capital
Autonomous republic (ASSR) or oblast center
Railroad
Road
An oblast is named only when its name differs from that of its administrative center.
0 100 200 Kilometers
0 100 200 Miles
Boundary representation is not necessarily authoritative.
801807 (R00110) 11-91

1991 - …

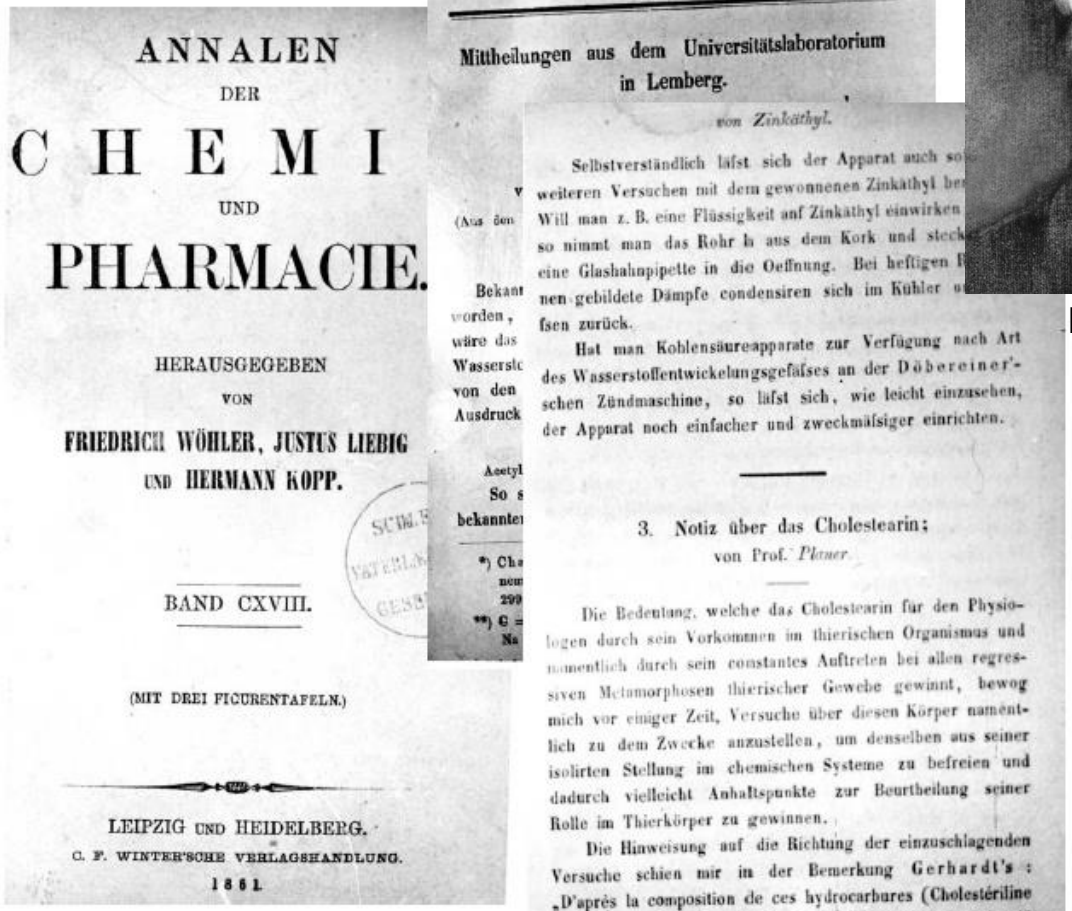

Ukraine
BELARUS
RUSSIA
POLAND
SLOVAKIA
HUNGARY
ROMANIA
MOLDOVA
SERBIA
Kamin'-Kashyrs'kyi
Kovel'
Sarny
Chornobyl'
Chernihiv
Shostka
Konotop
Luts'k
Rivne
Korosten'
Sumy
Kiev (Kyiv)
Pryluky
Novohrad-Volyns'kyi
Zhytomyr
Okhtyrka
L'viv
Sambir
Ternopil'
Bila Tserkva
Lubny
Kharkiv
Kupians'k
Khmel'nyts'kyi
Poltava
Stryi
Cherkasy
Kremenchuk
Lysychans'k
Luhans'k
Ivano-Frankivs'k
Vinnyts'kyi
Uzhhorod
hora Hoverla
6,761 ft.
(2,061 m)
Khust
Kamianets-Podil's'kyi
Uman'
Kramators'k
Horlivka
Kirovohrad
Pavlohrad
Chernivtsi
Pervomais'k
Dnipropetrovs'k
Donets'k
Kryvyi Rih
Kotovs'k
Nikopol'
Zaporizhzhia
Mariupol'
Mykolaiv
Melitopol'
Berdians'k
Kherson
Odesa
Sea of Azov
Krasnoperekops'k
Gulf of Karkinit
Crimea
Kerch
Izmail
Yevpatoriia
Feodosiia
Simferopol'
Sevastopol'
Yalta
Black Sea
Carpathian Mts.
Vistula
Dniester
Prut
Southern Bug
Dnieper
Donets
Desna
Don
24° E
28° E
32° E
36° E
40° E
52° N
48° N
44° N
0 100 Miles
0 100 Kilometers
© MAPQUEST.

Lviv Ivan Franko University

established 1661

Lviv Polytechnic University

established 1816


ANNALEN
DER
C H E M I
UND
PHARMACIE.
HERAUSGEGEBEN
VON
FRIEDRICH WÖHLER, JUSTUS LIEBIG
UND HERMANN KOPP.
BAND CXVIII.
(MIT DREI FIGURENTAFELN.)
LEIPZIG UND HEIDELBERG.
C. F. WINTER'SCHE VERLAGSHANDLUNG.
1861.

ANNALEN
DER
CHEMIE UND PHARMACIE.
CXVIII. Bandes erstes Heft.
Mittheilungen aus dem Universitätslaboratorium in Lemberg.

von Zinkäthyl.

Selbstverständlich läfst sich der Apparat auch so
weiteren Versuchen mit dem gewonnenen Zinkäthyl be
Will man z. B. eine Flüssigkeit auf Zinkäthyl einwirken
so nimmt man das Rohr h aus dem Kork und steck
eine Glashahnpipette in die Oeffnung. Bei heftigen
nen gebildete Dämpfe condensiren sich im Kühler u
fsen zurück.

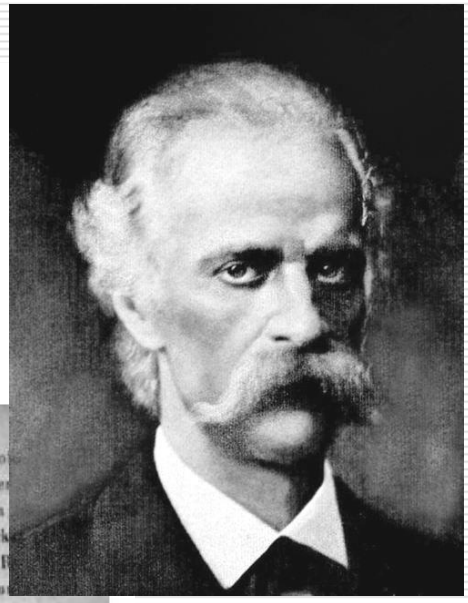
Hat man Kohlensäureapparate zur Verfügung nach Art des Wasserstoffentwickelungsgefäfses an der Döbereiner'schen Zündmaschine, so läfst sich, wie leicht einzusehen, der Apparat noch einfacher und zweckmäfsiger einrichten.

3. Notiz über das Cholestearin;
von Prof. *Planer*.

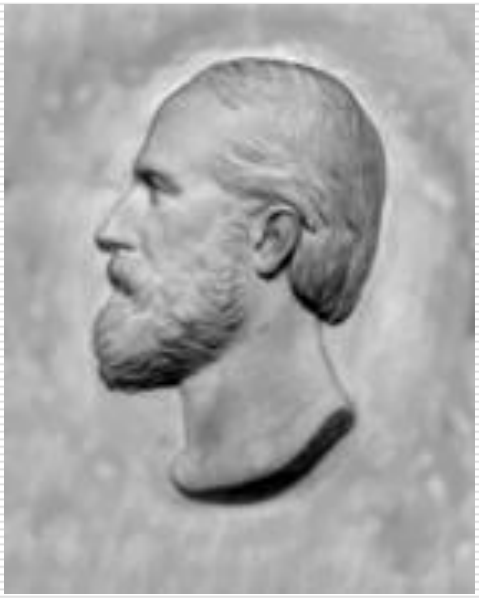
Die Bedeutung, welche das Cholestearin für den Physiologen durch sein Vorkommen im thierischen Organismus und namentlich durch sein constantes Auftreten bei allen regressiven Metamorphosen thierischer Gewebe gewinnt, bewog mich vor einiger Zeit, Versuche über diesen Körper namentlich zu dem Zwecke anzustellen, um denselben aus seiner isolirten Stellung im chemischen Systeme zu befreien und dadurch vielleicht Anhaltspunkte zur Beurtheilung seiner Rolle im Thierkörper zu gewinnen.

Die Hinweisung auf die Richtung der einzuschlagenden Versuche schien mir in der Bemerkung Gerhardt's: „D'après la composition de ces hydrocarbures (Cholestériline et Cholestérone) la cholestérine semble être une espèce d'alcool" zu liegen. (Traité de chim. org. par Gerhardt III, 739.)

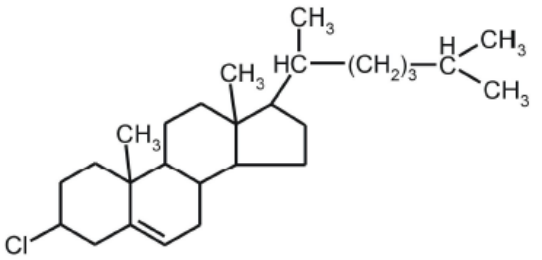
Nach dem Rathe Prof. Pebal's liefs ich Phosphorchlorid auf Cholestearin einwirken, wodurch ich eine Chlorver-

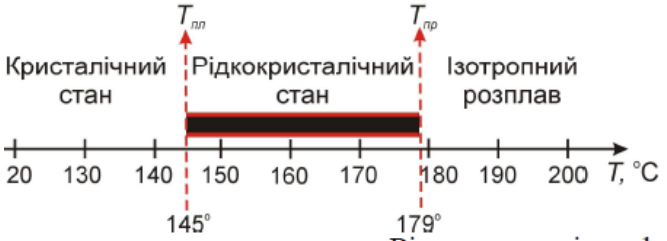


Leopold Pebal
(1826 – 1887)



Julis Planer
(1827 – 1881)





Хімічна формула холестерилхлориду. Рідкокристалічна фаза ефірів холестерину.

Department of Theoretical Physics, University of Lviv

Marian Smoluchowski
(1872 - 1917)

1899 - Privatdozent of mathematical physics

1899 - Chair of Theoretical Physics
(after the late Professor Oskar Fabian)

1900 - Extraordinary (associate) professor

1903 - Ordinary (full) professor

1906/1907 - Dean of the Philosophical Faculty

1913 – moved to Krakow

Prof. Maryan Ritter von Smolan Smoluchowski

While working at the University of Lviv, Marian Smoluchowski authored over 90 publications. The variety of subjects covered by these works is astonishing: Brownian motion, critical opalescence phenomenon, properties of viscous liquids, heat conduction in rarefied gases and in pulverized medium, etc.

However, major contributions was into development of the kinetic theory and molecular structure of matter

$$\Lambda = C\sqrt{2T}$$

4. *Zur kinetischen Theorie der Brownschen Molekularbewegung und der Suspensionen;* von *M. von Smoluchowski.*

[Bearbeitet nach einer am 9. Juli 1906 der Krakauer Akademie vorgelegten und demnächst in dem Bullet. Int. Crac. erscheinenden Abhandlung.]

§ 1. Die viel umstrittene Frage nach dem Wesen der von dem Botaniker Robert Brown 1827 entdeckten Bewegungserscheinungen, welche an mikroskopisch kleinen, in Flüssigkeiten suspendierten Teilchen auftreten, ist neuerdings durch zwei theoretische Arbeiten von Einstein [1]) wieder in Anregung gebracht worden. Die Ergebnisse derselben stimmen nun vollkommen mit einigen Resultaten überein, welche ich vor mehreren Jahren in Verfolgung eines ganz verschiedenen Gedankenganges erhalten hatte, und welche ich seither als gewichtiges Argument für die kinetische Natur dieses Phänomens ansehe. Obwohl es mir bisher nicht möglich war, eine experimentelle Prüfung der Konsequenzen dieser Anschauungsweise vorzunehmen, was ich ursprünglich zu tun beabsichtigte, habe ich mich doch entschlossen, jene Überlegungen nunmehr zu veröffentlichen, da ich damit zur Klärung der Ansichten über diesen interessanten Gegenstand beizutragen hoffe, insbesondere da mir meine Methode direkter, einfacher und darum vielleicht auch überzeugender zu sein scheint als jene Einsteins.

Dem Mangel einer direkten experimentellen Verifikation suche ich teilweise wenigstens durch eine zusammenfassende Übersicht der bisher bekannten Versuchsresultate abzuhelfen, welche im Verein mit einer kritischen Analyse der verschiedenen Erklärungsversuche deutliche Hinweise darauf zu geben scheint, daß das Brownsche Phänomen in der Tat mit den theoretisch vorauszusehenden Molekularbewegungen identisch ist. Den Schluß bilden einige Bemerkungen über die Suspensionen

1) A. Einstein, Ann. d. Phys. **17.** p. 549. 1905; **19.** p. 371. 1906.

It worth to mentioning that Smoluchowski was not the only Lviv researcher to contribute to the study of the Brownian motion.

Back in 1881, Lukasz Bodaszewski, then an assistant at the Higher Polytechnic School in Lviv, observed the Brownian motion in gases using an enhanced microscope of his own construction.

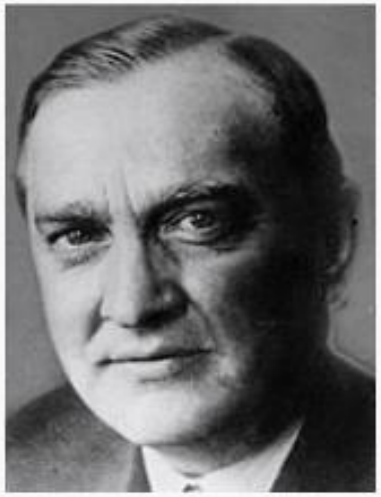
Marian Smoluchowski referred to Lukasz Bodaszewski'observations in his works and it is quite likely that two scientists met in Lviv.

Lukasz Bodaszewski
(1849–1908)

Rovenchak A. and Trokhymchuk A. *From Brownian Motion to Molecular Simulations*, MATHEMATICAL MODELING AND COMPUTING, Vol. 5, No. 2, pp. 99–107 (2018)

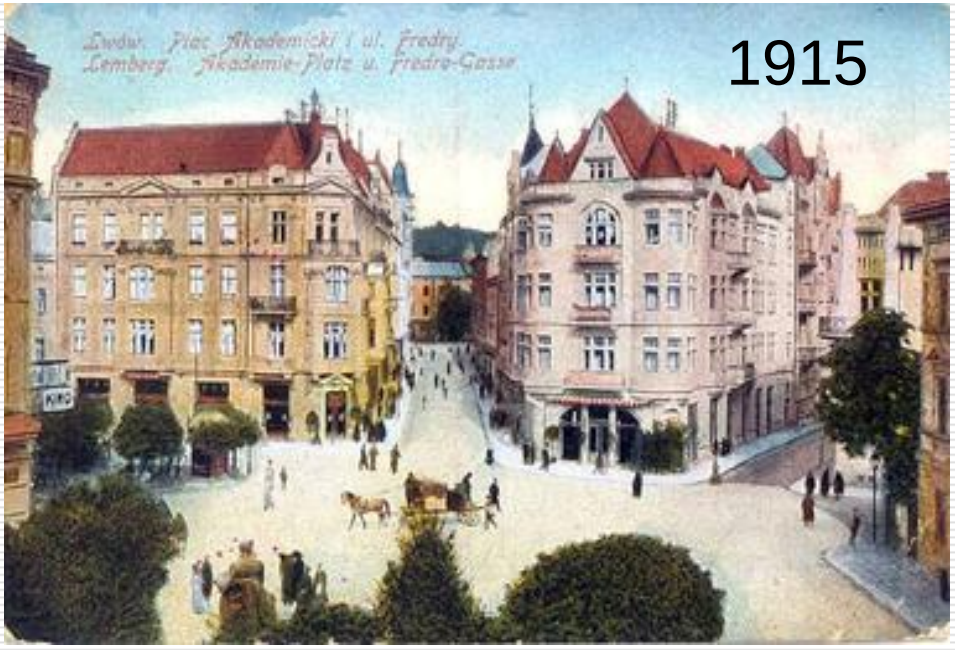
LVIV SCHOOL OF MATHEMATIC

Stefan Banach

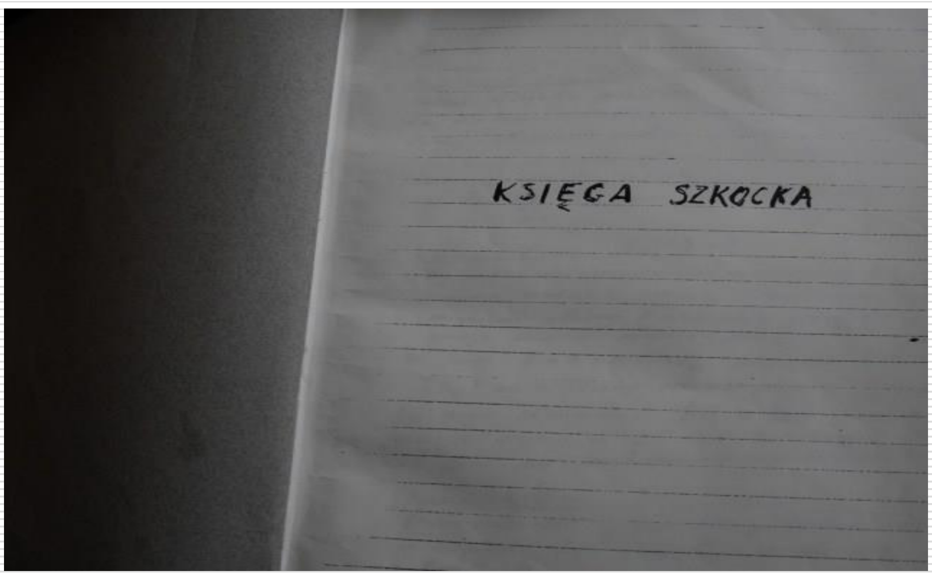


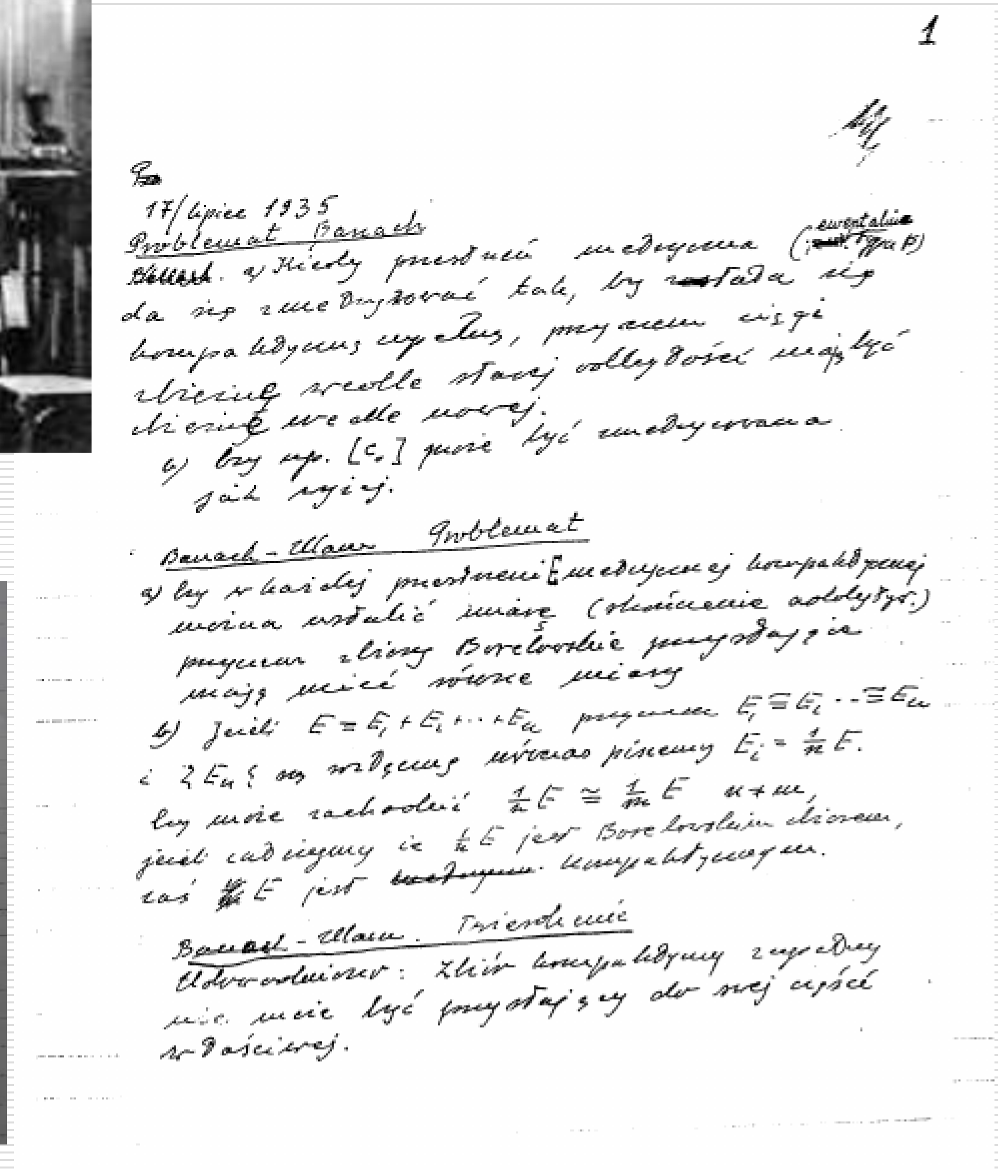
Born	March 30, 1892 Kraków, Grand Duchy of Kraków, Austria-Hungary (today Poland)
Died	August 31, 1945 (aged 53) Lviv, Ukrainian SSR, Soviet Union (today Ukraine)
Nationality	Polish
Fields	Mathematics
Institutions	University of Lwów
Alma mater	Technical University of Lwów
Doctoral advisor	Hugo Steinhaus
Doctoral students	Stanisław Mazur
Other notable students	Stanislaw Ulam
Known for	Banach–Tarski paradox Banach–Steinhaus theorem Functional analysis
Notable awards	Memberships: Academy of Sciences of the Ukrainian SSR, Polish Academy of Learning

Scottish Cafe in Lviv (Szkocka Café)



Scottish Book
(KSIEGA SZKOCKA)





The Scottish Book: A Collection of Problems. An edited translation of a notebook kept at the Scottish Cafe for the Lwow Section of the Societe Polonaise de Mathematiques. Privately mimeographed and distributed by S. M. Ulam in 1957. Reprinted as Los Alamos Scientific Laboratory report LA-6832, 1967.

Mazur & Ulam in Lviv
1938

Fields	Mathematics
Institutions	Institute for Advanced Study Harvard University University of Wisconsin Los Alamos National Laboratory University of Colorado University of Florida
Alma mater	Lwów Polytechnic Institute
Doctoral advisor	Kazimierz Kuratowski
Doctoral students	Paul Kelly
Known for	Key mathematical formulations in the fields of Physics, Computer Science, and Biology Teller–Ulam design Monte Carlo method Fermi–Pasta–Ulam problem Nuclear pulse propulsion

Stanisław Ulam

Stanisław Ulam

Born	Stanisław Marcin Ulam 13 April 1909 Lemberg, Austria-Hungary (now Lviv, Ukraine)
Died	13 May 1984 (aged 75) Santa Fe, New Mexico
Citizenship	American (after 1941)
Nationality	Polish

Monte Carlo

✓ Credit for inventing the Monte Carlo method often goes to Stanislaw Ulam, a mathematician who worked for John von Neumann on the United States' Manhattan Project during World War II.

✓ He conceived of the Monte Carlo method in 1946 while pondering the probability of winning a game of solitaire.

✓ After attempting to solve this problem with pure combinatorial calculations, he wondered if it might be simpler to play multiple hands of solitaire and observe the frequency of wins.

✓ This lead Ulam to consider how problems of neutron diffusion and other questions of mathematical physics might be represented in a form interpretable as a succession of random operations.

Ulam's ID badge
(photo from Los Alamos)

List of Mathematicians from the Scottish Book

1. Akexandroff
2. Auerbach
3. Banach
4. Bogolubov (Problem 183)
5. Fréchet
6. Infeld
7. Kac
8. Kaczmarz
9. Kuratowski
10. Łomnicki
11. Mazur
12. Marcinkiewicz
13. Nikliborc
14. Orlicz
15. Ruziewicz
16. Schreier
17. Schauder
18. Sternbach
19. Steinhaus
20. Ulam
21. Zygmunt
22. Sierpiński
23. Eilenberg
24. Wavre
25. Ward (Problems 156,157)
26. Stoilow (Problem 158)
27. von Neumann (Problem 163)
28. Szpilrajn (Problems 169,170)
29. Eidelheit (Problems 172-174,176,188)
30. Borsuk (Problem 175)
31. Offord (Problem 179)
32. Kampe de Feriet (Problem 180)
33. Knaster (Problem 182)
34. Saks (Problem 184,185)
35. Szpilrajn (Problem 191)
36. Sobolew (Problem 188)
37. Eilenberg
38. Eidelheit (1940.11.27)
39. Fermant (Problem 189)
40. Lusternik (Problem 190)
41. Knaster

— cyklicznych o wymiarze $k \leq n-2$. (mete jame).

183. Problemat Bogrlabova 8 lutego 1940 r.

Etant donné un groupe compact, connexe et localement connexe des transformations de l'espace euclidien n-dimensionnel.

Démontrer (ou donner un Gegenbeispiel) qu'on peut introduire dans cet espace des telles coordonnées que les transformations du groupe seront linéaires.

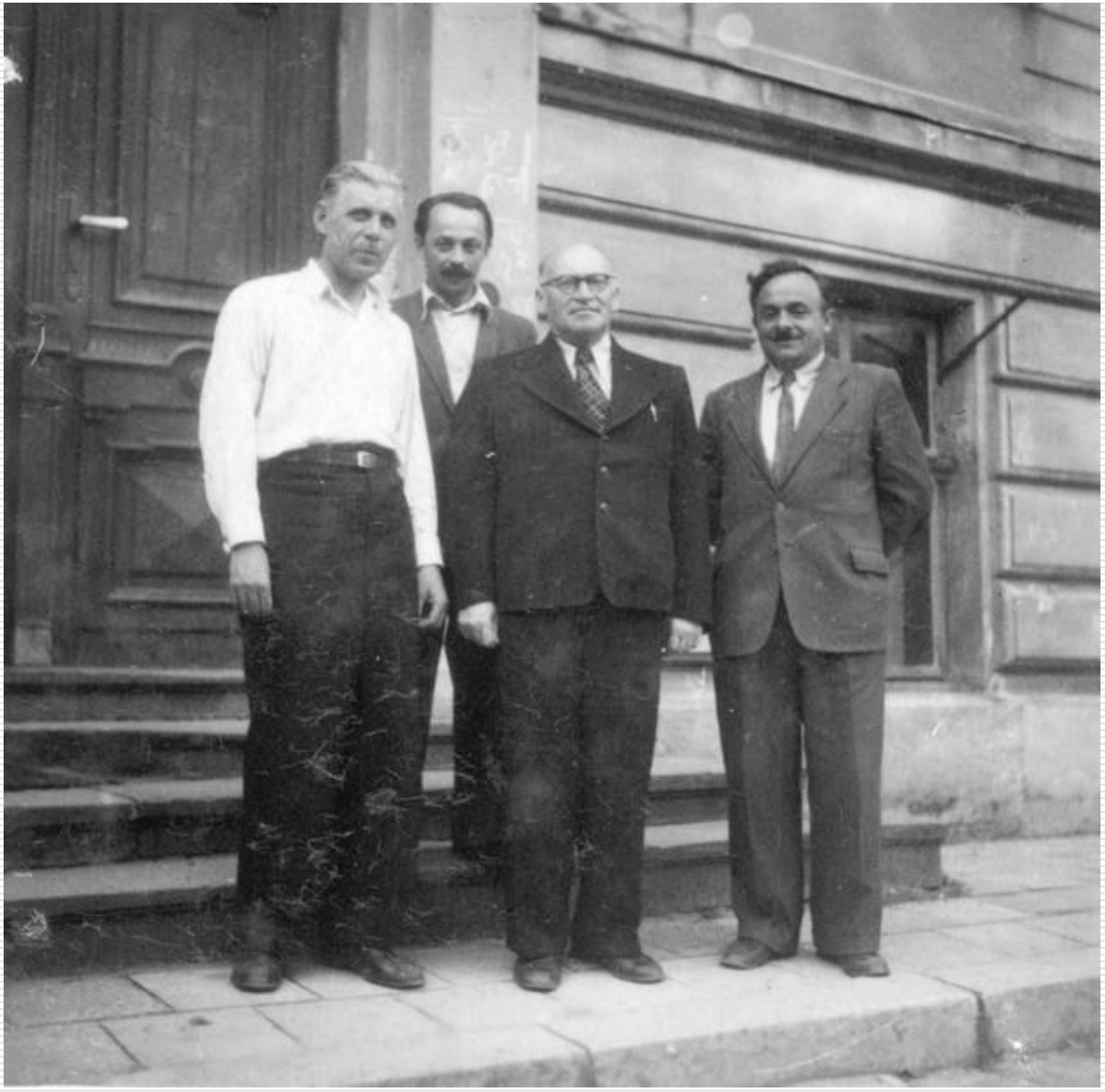
(plaszka kuniaku)

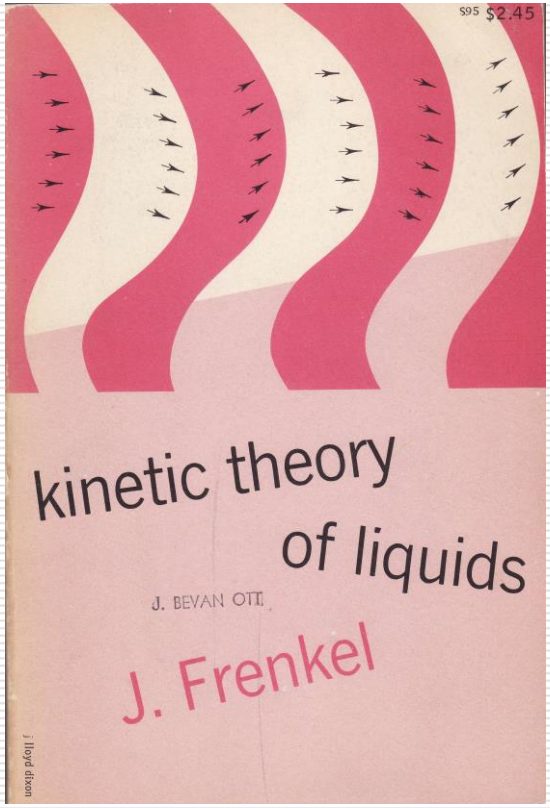
184. Problemat. S. Saks. 8. II. 1940 r.

Department of Theoretical Physics, University of Lviv

Profs. W. Milianczuk, N.N. Bogolyubov and A. Yu. Glauberman (middle 1950s)

Department of theoretical Physics, University of Lviv





Profs. O.I. Andriyevski, A. Yu. Glauberman, J. I. Frenkel, W. Milianczuk (1949)

Department of Theoretical Physics, University of Lviv

Ihor Yukhnowskii (1945)

Department of theoretical Physics, University of Lviv

I.R. Yukhnowskii and A.Yu. Glauberman (1953)

Т. 22. Журнал экспериментальной и теоретической физики. Вып. 5
1952

К СТАТИСТИЧЕСКОЙ ТЕОРИИ КОНЦЕНТРИРОВАННЫХ РАСТВОРОВ СИЛЬНЫХ ЭЛЕКТРОЛИТОВ. I

А. Е. Глауберман и *И. Р. Юхновский*

V. 22 Journal of Experimental and Theoretical Physics, Issue 5

On the Statistical Theory of a Dense Electrolyte Solutions. Part I

A.Yu. Glauberman and I.R. Yukhnowskii

Метод, развитый Боголюбовым [1] для статистических систем взаимодействующих частиц, позволяет построить статистическую теорию концентрированных растворов сильных электролитов, лишенную принципиальных недостатков, присущих теории Дебая—Гюккеля. Область применимости этой теории охватывает значения концентраций, соответствующие реальным растворам, в противоположность теории Дебая, приближенно справедливой лишь для предельно малых концентраций.

Как было показано Боголюбовым [1], при описании взаимодействия ионов при помощи закона Кулона можно определить лишь нулевое приближение бинарной функции распределения, которое при выбранном Боголюбовым чисто-кулоновском потенциале взаимодействия не выводит за рамки простой теории Дебая, получение же высших приближений оказывается, вообще говоря, лишенным смысла, так как свойство расходимости при малых расстояниях между частицами, усиливается [1].

Общие квантово-механические соображения, с одной стороны, и полуэмпирические данные, с другой [1], приводят к потенциалу, удовлетворительно описывающему взаимодействие двух ионов вида:

$$\Phi = (e^2 / r)\,[1 - A(r)\,e^{-\alpha r}], \tag{1.1}$$

где $\alpha \gg 1$, $A(r)$ — функция, стремящаяся к единице при $r \to 0$. При r, достаточно далеких от нуля (однако, вообще говоря, малых) этот потенциал учитывает обменное и поляризационное взаимодействия, а на расстояниях, близких к нулю, обеспечивает отсутствие чисто-кулоновского члена и, следовательно, качественно, учитывает силы отталкивания. Функция $A(r)$ может быть взята хотя бы в следующем виде:

$$A(r) = 1 + a_1 r + \cdots + a_n r^n. \tag{1.2}$$

Условие $A(r) \to 1$ при $r \to 0$ является не тольке формальным, но и физическим требованием, так как кулоновский член в явном виде должен отсутствовать при достаточно малых расстояниях между частицами [2].

Т. 22. Журнал экспериментальной и теоретической физики. Вып. 5

1952

К СТАТИСТИЧЕСКОЙ ТЕОРИИ КОНЦЕНТРИРОВАННЫХ РАСТВОРОВ СИЛЬНЫХ ЭЛЕКТРОЛИТОВ. II

А. Е. Глауберман и *И. Р. Юхновский*

V. 22 Journal of Experimental and Theoretical Physics, Issue 5

On the Statistical Theory of a Dense Electrolyte Solutions. Part II

A.Yu. Glauberman and I.R. Yukhnowskii

молекул растворенного вещества, влияние растворителя учитывается путем введения в закон взаимодействия ионов макроскопической диэлектрической постоянной ε; распределение ионов характеризуется шаровой симметрией [1]. Раствор в целом удовлетворяет условию нейтральности:

$$\sum_a e_a N_a = 0, \tag{1.1}$$

где a, равное $1, 2, \ldots s$, нумерует сорта ионов и e_a означает заряд иона сорта a; N_a — число ионов этого сорта. Взаимодействие двух ионов друг с другом описывается взаимным потенциалом, имеющим вид [1,2]:

$$\Phi_{ab}(r) = \frac{e_a e_b}{\varepsilon r}(1 - e^{-\alpha r}), \tag{1.2}$$

$$kT \ln f_i = -\frac{1}{2\beta\varepsilon}\left(e_i^2 - \frac{\gamma e I}{1+\gamma c}\right)\left(1 - \frac{1}{\sqrt{1+2\beta\varkappa}}\right), \qquad (2.9)$$

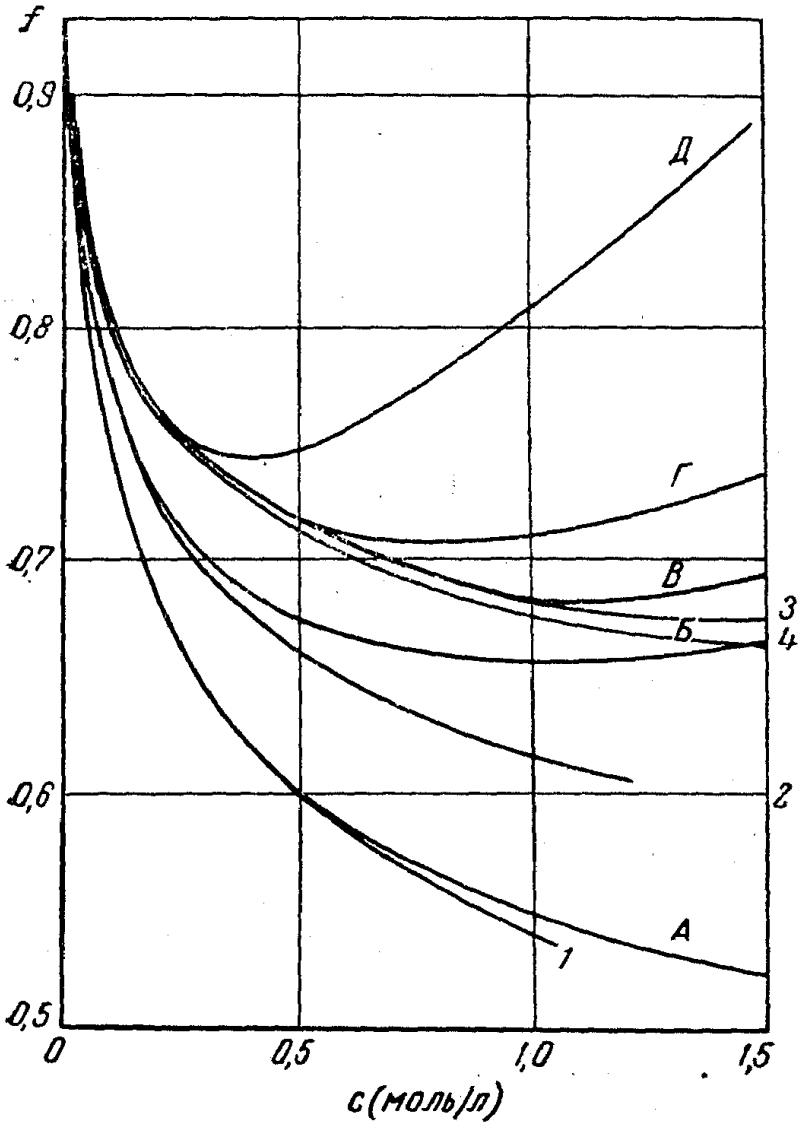
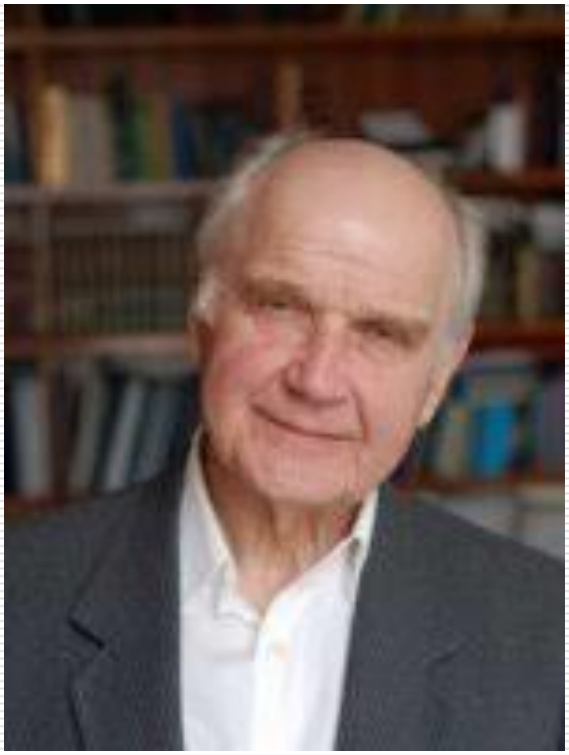


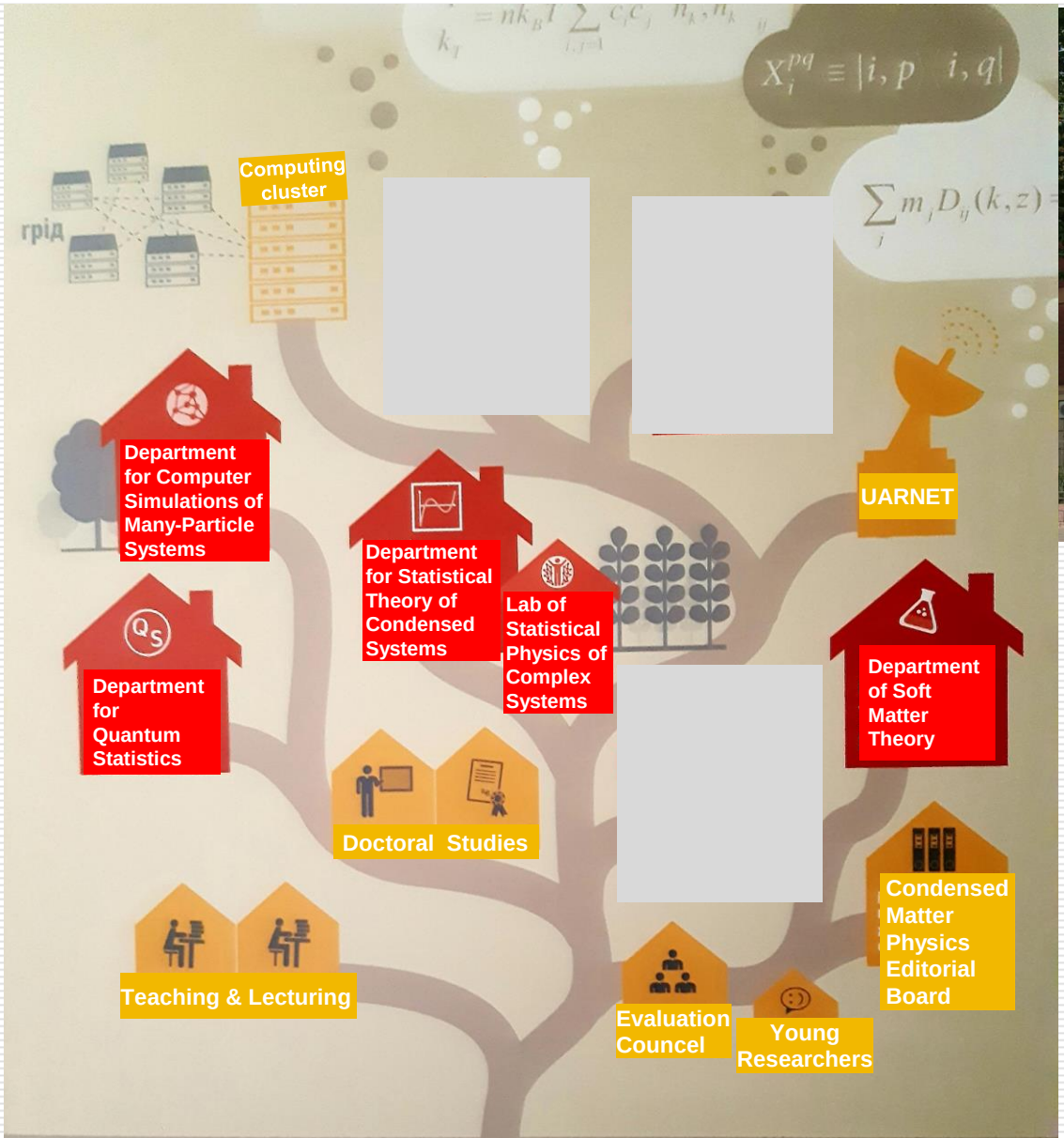
Рис. 1. Зависимость коэффициента активности f от концентрации c. *1*, *2*, *3*, *4* — теоретические кривые для значений $\beta = 1{,}85 \times \times 10^{-8}$; $2{,}90 \cdot 10^{-8}$; $4{,}60 \cdot 10^{-8}$; $4{,}50 \cdot 10^{-8}$ соответственно. Экспериментальные кривые соответствуют: *А* — LiOH: *Б* — NaOH; *В*, *Г* — NaBr и *Д* — HCl



Prof. Igor Yukhnowskii

- 1954 – PhD thesis “Radial distribution function of the system interacting charged particles” (supervisor Prof. A.Yu. Glauberman)
- 1965 – DrSci thesis “Statistical theory of the system of charged particles”
- 1969 – Head of the Department of Statistical Theory of Condensed Systems @ Institute for Theoretical Physics of the Academy of Sciences of Ukr. SSR
- 1990 – 2006 Director of the Institute for Condensed Matter Physics

Institute for Condensed Matter Physics of the Natl. Acad. Sci. of Ukraine (as of 2016)



- 83 peoples
- 7 administration
- 63 researchers
- 49 PhD & DrSci

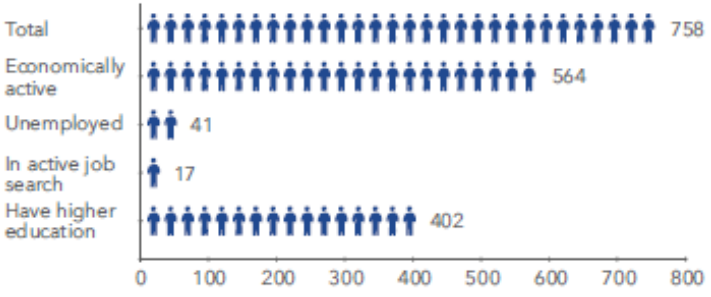
Scientific Meetings organized by Institute for Condensed Matter Physics of the Natl. Acad. Sci. of Ukraine

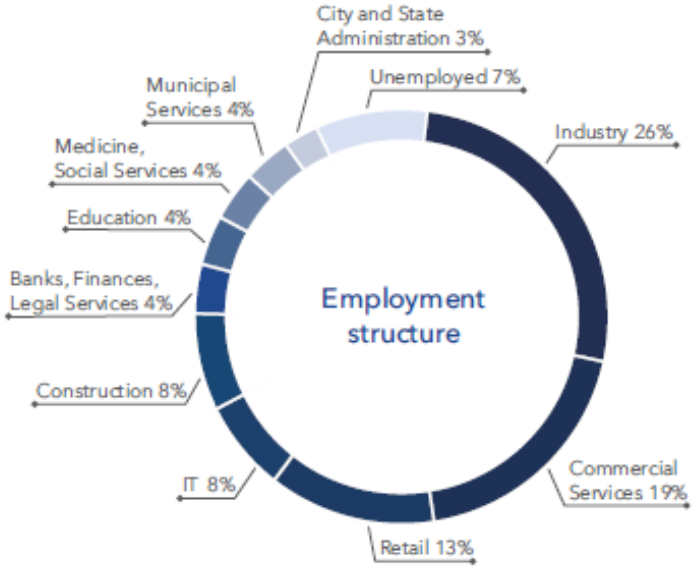
- Physics of Ionic Solvation, May 30 – June 1, 1983
- Soviet-Italian Simposium on the Mathematical Problems of Statistical Physics, Sept 30 – Oct 11, 1985
- Ukrainian-French Symposium "Condensed Matter: Science & Industry", Feb 20-27, 1993
- NATO ARW on Ionic Soft Matter "Novel Trends in Theory & Applications", Apr 14-17, 2004
- NATO ARW on Ionic Soft Matter "Size Effects in Non-Linear Ferroics", Oct 19-22, 2004
- 1st Conference on Statistical Physics: "Modern Trends & Applications", Aug 28-30, 2005
- Planer-Smoluchowski Soft Matter Workshop on Colloidal Suspensions, June 22, 2009
- 3rd Conference on Statistical Physics: "Modern Trends & Applications", June 23-25, 2009
- 28th Meeting of European Molecular Liquid Group on Complex Liquids, Sept 5-9, 2010
- 36th Conference Middle European Cooperation in Statistical Physics (MECO, Apr 5-7, 2011
- Planer-Smoluchowski Soft Matter Workshop on Liquid Crystal Colloids, Oct 5-7, 2011
- 4th Conference on Statistical Physics: "Modern Trends & Applications", July 3-6, 2012
- Ulam Computer Simulation Workshop, June 21-24, 2017
- 5th Conference on Statistical Physics: "Modern Trends & Applications", July 3-6, 2019

City of Lviv today

PEOPLE

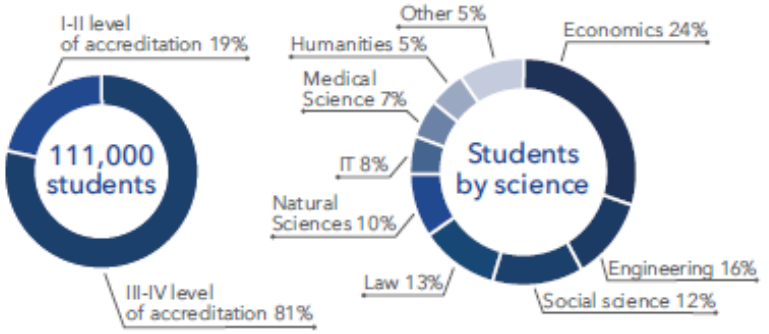
Total population, '000 people





Source: Lviv Investment Office, 2019

EDUCATION



Universities (III-IV level of accreditation), students

Lviv Polytechnic National University	25,835
Ivan Franko National University of Lviv	19,160
Danylo Halytsky Lviv National Medical University	4,848
Lviv National Agrarian University	4,778
Lviv State University of Internal Affairs	4,646
Lviv National University of Veterinary Medicine and Biotechnologies	3,301
Ukrainian National Forestry University	3,234
Hetman Petro Sahaidachny National Army Academy	2,973
Lviv University of Trade and Economics	2,904
Lviv State University of Physical Culture	2,712
Ukrainian Academy of Printing	2,507
Lviv State Financial Academy	2,500
Lviv State University of Life Safety	1,962
Ukrainian Catholic University	1,459
Lviv National Academy of Arts	1,079
10 other small universities	6,329
Total	90,227

Source: City Institute, 2018

IT INDUSTRY

317	IT companies in Lviv
21%	of city GRP
21,000	IT specialists
56%	software engineers
99.6%	speak English
4,500	IT specialists graduate annually
28%	predicted annual growth of IT industry
3,000+	participants in IT Arena annual event

Source: Lviv IT Cluster, 2019

Companies from The Global Outsourcing 100 present in Lviv:

softserve* eleks* infopulse

SIGMA N-iX

CIKLUM epam intellias

*HQ in Lviv

LVIV IT CLUSTER
0800 300 331
info@itcluster.lviv.ua
itcluster.lviv.ua

Material design assisted by machine learning

M. Druchok[a,b], D. Yarish[a], O. Gurbych[a] and M. Maksymenko[a]

[a] *Softserve Inc., 2D Sadova Str., 79021 Lviv, Ukraine*
[b] *Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Str., 79011 Lviv, Ukraine*

Efficient design and screening of the novel molecules is a major challenge in drug and material design. In this contribution we present a multi-stage pipeline in which several deep neural networks are used to generate and validate novel molecular structures with the desired properties. Here the Autoencoder network is trained on existing structures to convert discrete molecular representations to continuous vector representation and reconstruct back the structure for a given vector in that space. An Attention-based Sequence to Sequence model "spell-checks" errors in the generated structures, while a fully connected Regressor type network is trained to predict desired molecular descriptors. In addition, we extend the scheme by adding few steps assessing the quality of the generated molecules. To this end, we use oversampling techniques in the continuous space to generate candidate structures and compute Synthetic accessibility score to assess the likeliness of the molecule synthesis.


Thank You !
Thank You !
Thank You !