University of Science and Technology of China , Dec. 2, 2011，Hefei

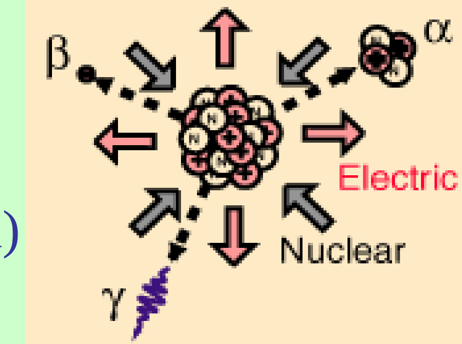
A multi-scale microscopic dynamical model of heavy ion interacts with biomolecules

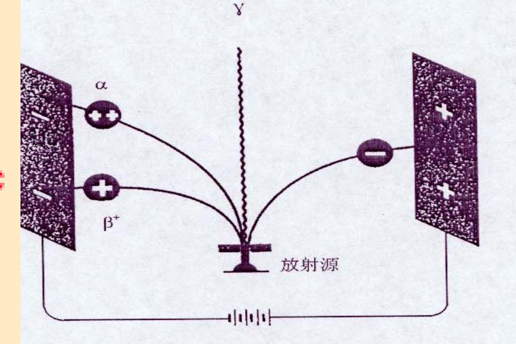
Feng-Shou Zhang (张丰收)

College of Nuclear Science and Technology
Beijing Normal University
Beijing, China
Tel: 010-6220 5602
Fax: 010-6223 1765
E-mail: fszhang@bnu.edu.cn
http://lenp.bnu.edu.cn/hkxyweb/zhangfengshou.htm

1896 H. Becquerel, from x-rays to

U rays? (α,$\beta^{\pm}$,γ,Heavy Ion)





1898 M. and P. Curie,

Polonium and Radium, Radioactivity

1911 Ernest Rutherford,

theoretical picture

of an atom

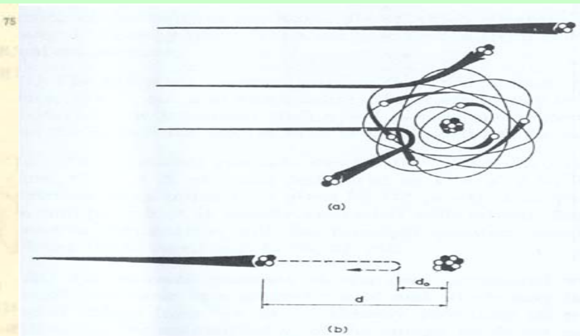


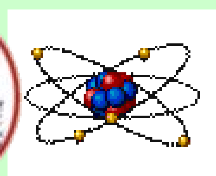
Fig. 1.2. Deflection of α-particles by atomic nuclei.

1919 E. Rutherford,

the first nuclear reaction in lab , $^{14}N + \alpha \text{---->} {}^{17}O + p$

1931 W.Pauli proposed neutrino

1932 J. Chadwick discoveried neutron



$$ {}^{9}_{4}Be + {}^{4}_{2}He \longrightarrow {}^{12}_{6}C + {}^{1}_{0}n $$

1932 J.Cockcroft and E.Walton accelerator

1934 I. and F. Joloit-Curie, artificial radioactive isotope

$$ {}^{27}_{13}Al + {}^{4}_{2}He \longrightarrow {}^{30}_{15}P + {}^{1}_{0}n, \quad {}^{30}_{15}P \xrightarrow{\beta^{+}} {}^{30}_{14}Si $$

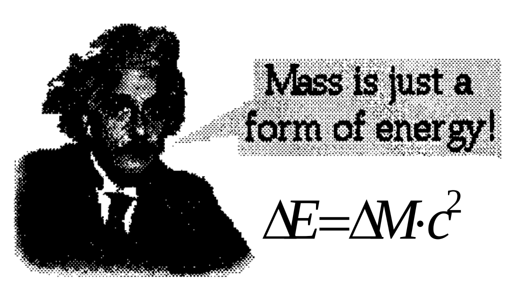
1935 H. Yukawa Pion meson theory

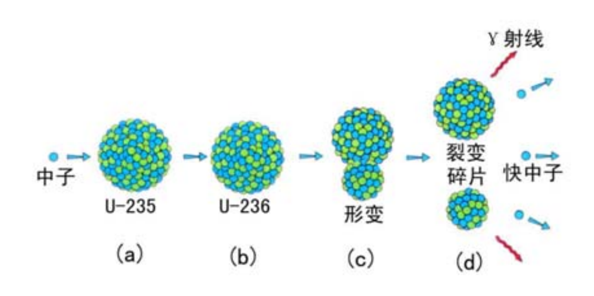
1936 N. Bohr Compound nuclei model

1938 O. Hahn and F. Starssmann, fission (energy: 200 MeV)

1 Kg (U)=

2.7×10^{6} Kg (coal)





1939 N. Bohr and J. Wheeler, liquid drop model for fission

1942 E. Fermi Reactor, Nuclear energy (52 tons ^{235}U)

1945 J. R. Oppenheimer, Atomic nuclear bomb

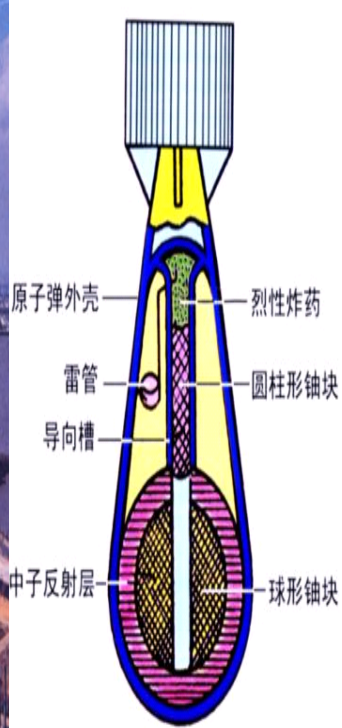
1948 M. Mayer and J. H. Jensen, Shell model

1952 E. Teller Hydrogen bomb

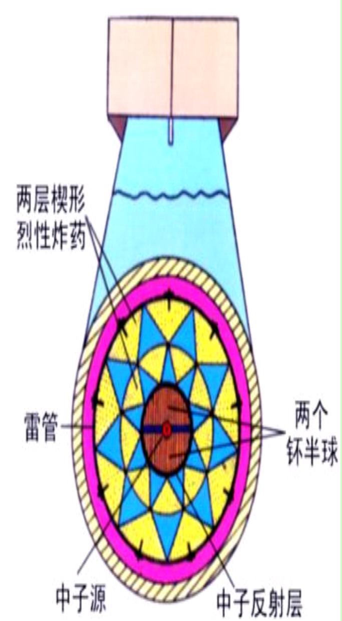
$$4\,{}^{1}H \longrightarrow {}^{4}He + 2\beta^{+} + 2\gamma + 2\nu + 26.7\,\mathrm{MeV}$$

1953 A. Bohr and B. Mottelson, Nuclear collective Model

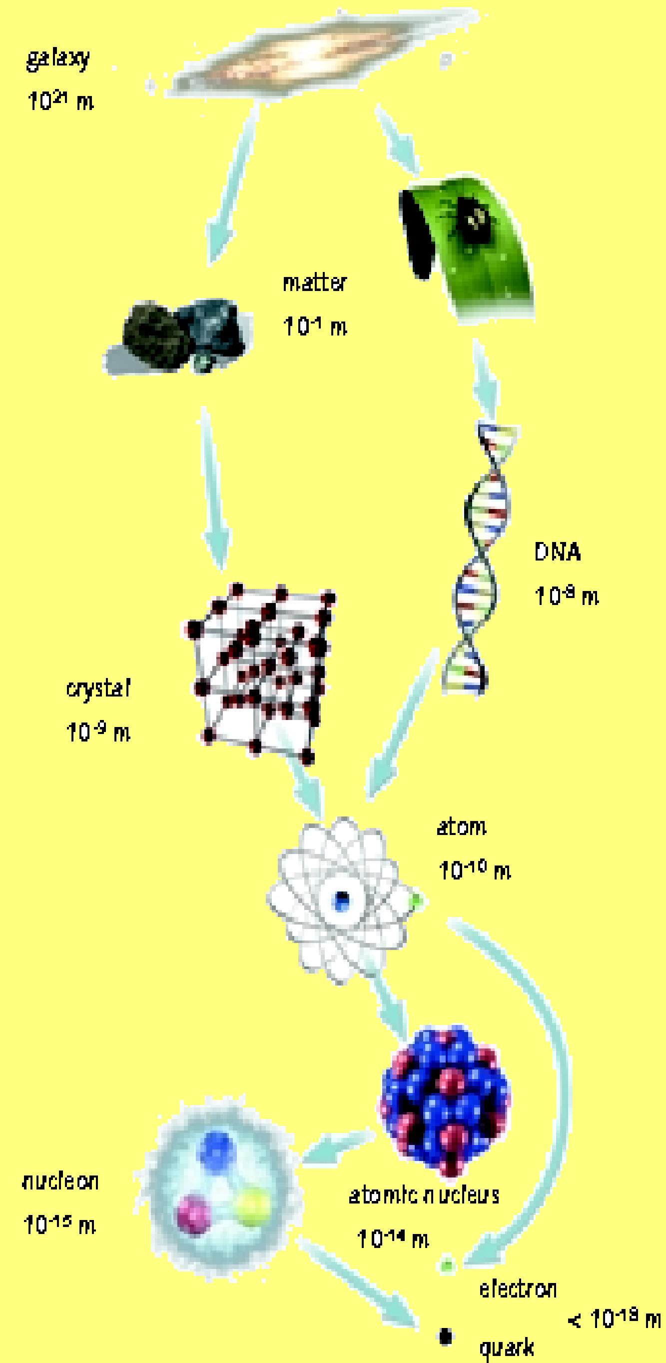
Nuclear Science and Technology



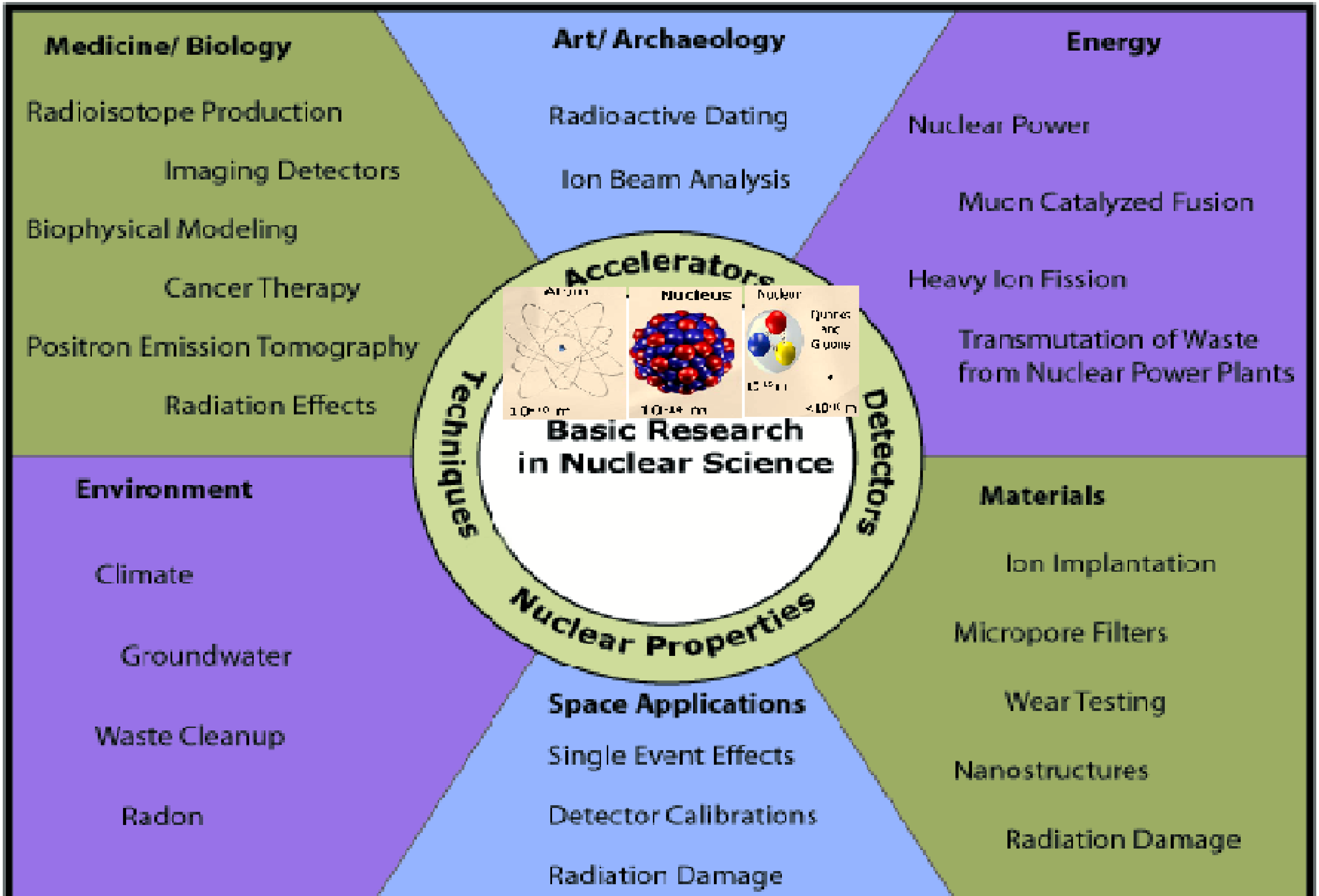
“枪式”原子弹结构原理图



“内爆式”原子弹结构原理图



Applications of Nuclear Science

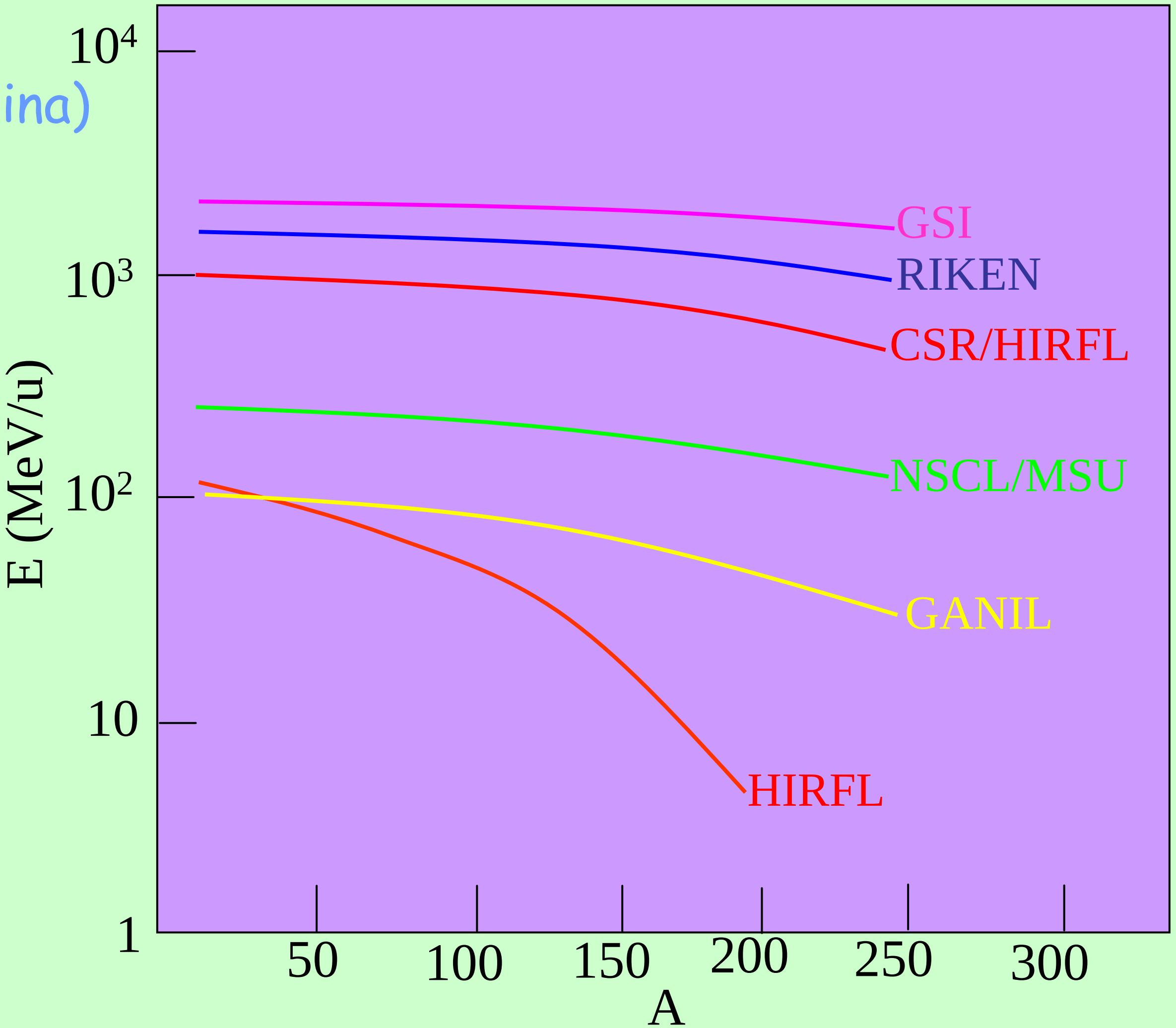


Heavy-Ion Accelerators at Intermediate Energies

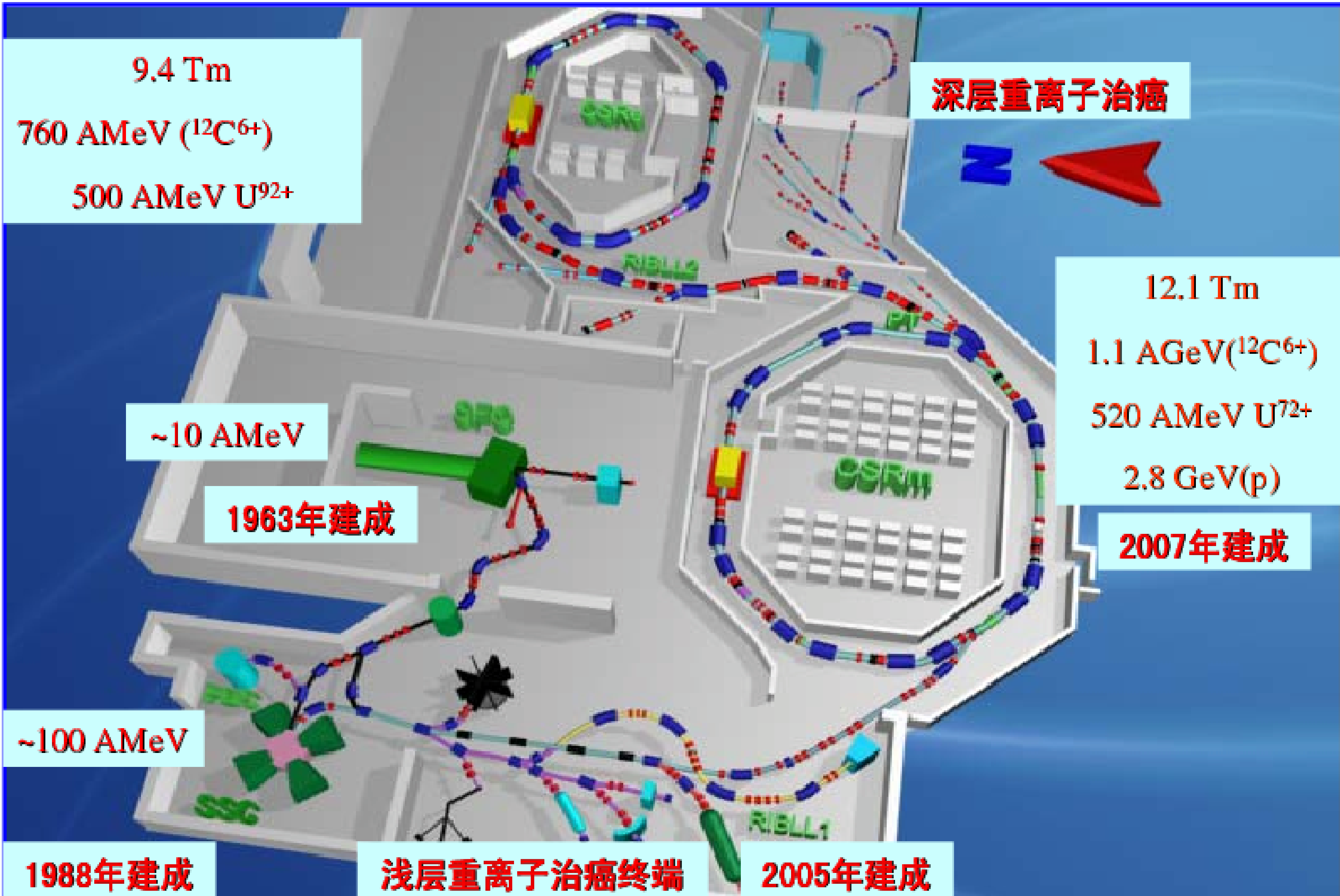
1. HIRFL, CSR/HIRFL (China)
2. GANIL (France)
3. GSI (Germany)
4. NSCL/MSU
5. RIKEN (Japan)

Dubna, LBL, ORNL, TAMU, INFN, KVI,…

BNL, CERN



HIRFL-CSR


9.4 Tm
760 AMeV ($^{12}C^{6+}$)
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Outline

1. Introduction

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    2.1 Cancer therapy

    2.2 Seed breeding

    2.3 Space radiation

    2.4 Problems

3. A Multi-scale microscopic dynamical model

4. Conclusions

Radiation is everywhere, all the time

Natural radiation from space and earth（15,000,000,000 years！）

medical examination（x-rays, neutron, …）

plant

animal

human being

Modification, evolution (Charles Robert Darwin), death…

A Simple history

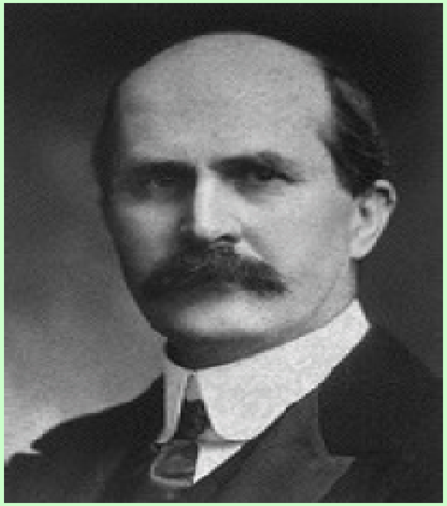
1. 1895， Wilhelm Konrad Roentgen discovered x-rays, won a 1901 Nobel Prize

2. γ-rays, e^-, n, π, …

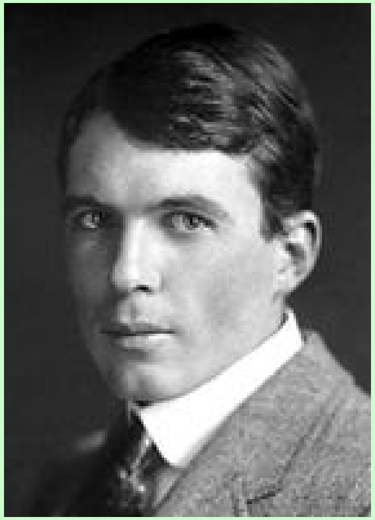
3. Proton and heavy ions

In 1903, William Henry Bragg found a peak as α particle penetration in materials (Bragg peak), shared the 1915 Nobel Prize with his son

Bragg peak - discovered in 1904



William Henry Bragg



William Lawrence Bragg

1. Bragg and Kleeman, On the ionization curves of radium, Philosophical Magazine, S.6, 8(1904)726
2. Bragg, Die alpha-Strahlen des Radiums, Jahrbuch der Radioaktivitat und Elektronik, 2(1905)4.
3. Bragg and Kleeman, On the alpha particles of radium, and their loss of range in passing through various atoms and molecules, Philosophical Magazine, S.6, 10(1905)318

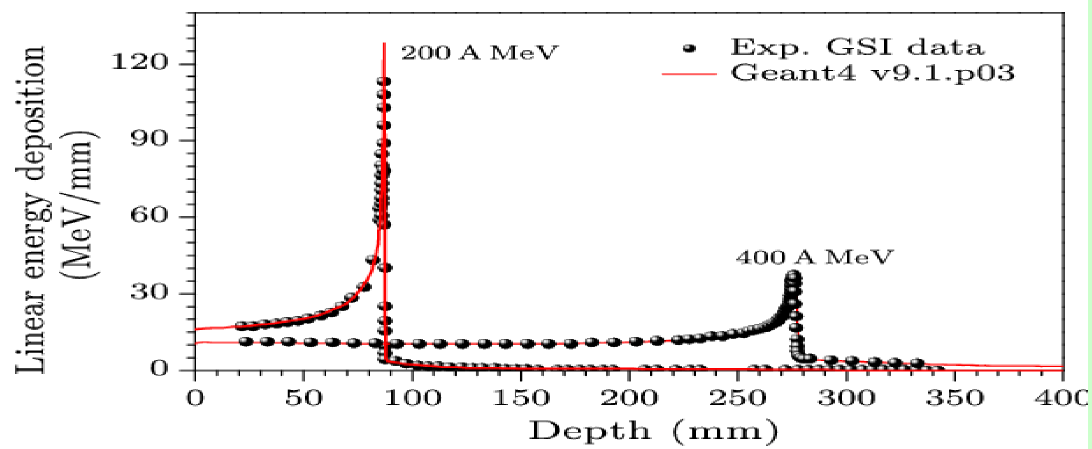


Fig. 1. Average linear energy deposition by ^{12}C ions in water. The beam energies are given in the boxes. GEANT4 calculations are shown by histograms; experimental data from GSI (Sihver *et al.* 1998)[27] are shown by circles.

The Lawrence Brothers

E.O. Lawrence (right) poses with his sixty inch cyclotron.

Ernest Orlando Lawrence (1901-58)

1931 The first cyclotron was produced by Lawrence and Livingston. It was 4.5 inches in diameter and used 1800V to produce 80KeV protons.

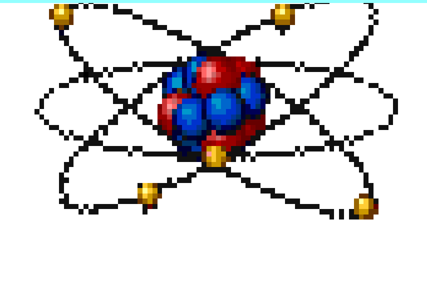
1939 EOL was awarded the Nobel Prize for his invention of the cyclotron.

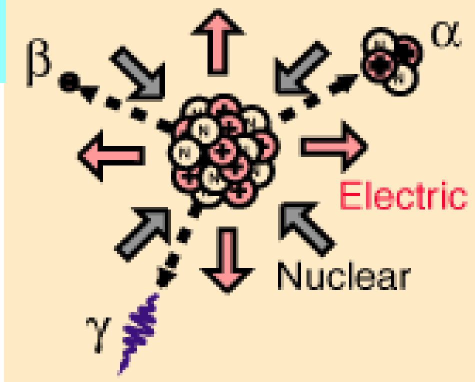
John H. Lawrence (1903-1991)

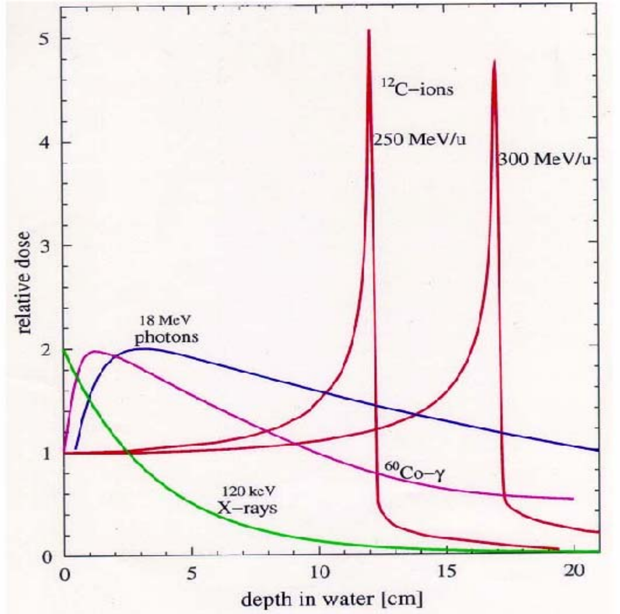
Ernest's younger brother John was a Doctor of Medicine. He came to the Radiation Laboratory in '35. John Lawrence was the first to treat cancer with cyclotrons when, in 1954, he began irradiating the pituitaries of patients with metastatic breast cancer.

John H. Lawrence using the 60 inch cyclotron to treat a patient with neutrons.

x,γ, n,p,HI,…

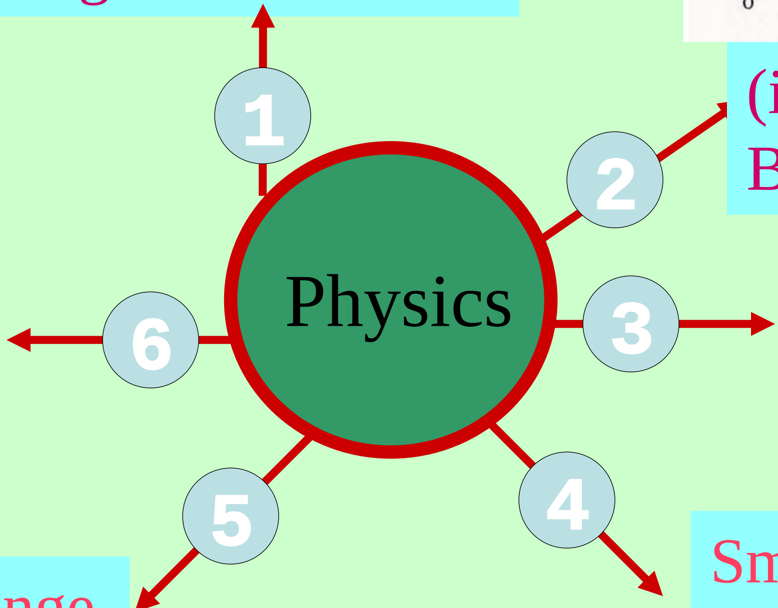






Strong electro-magnetic radiation

(inverse dose profile) Bragg Curve



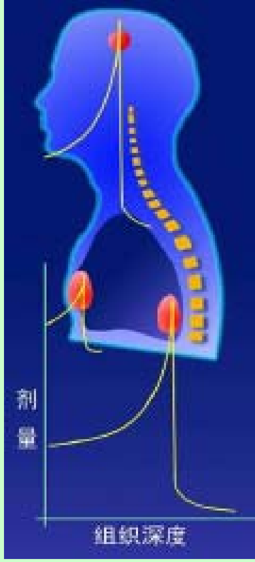
Small range-straggling

Small lateral scattering

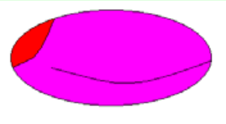
Determinate range

Beam verification

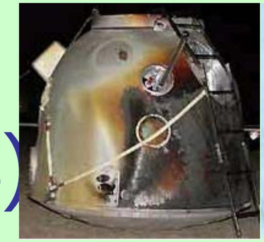
Physical advantages



1. Proton and HI therapy
   EU, Japan, China, USA,…

2. Seed breeding  

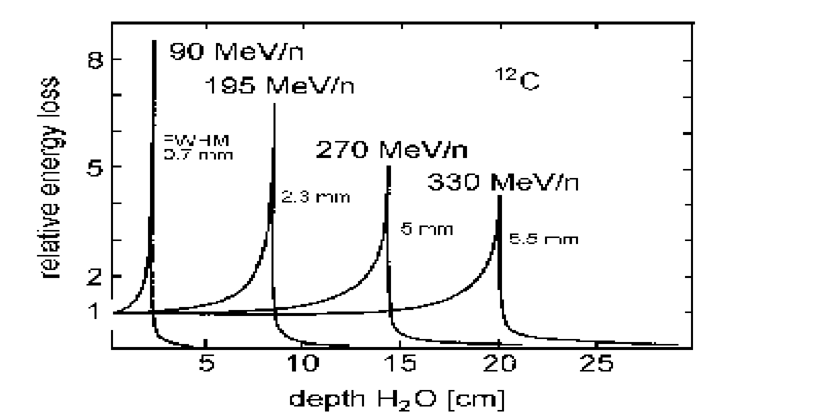
3. Radioprotection
   (Space, power stations, hospitals)

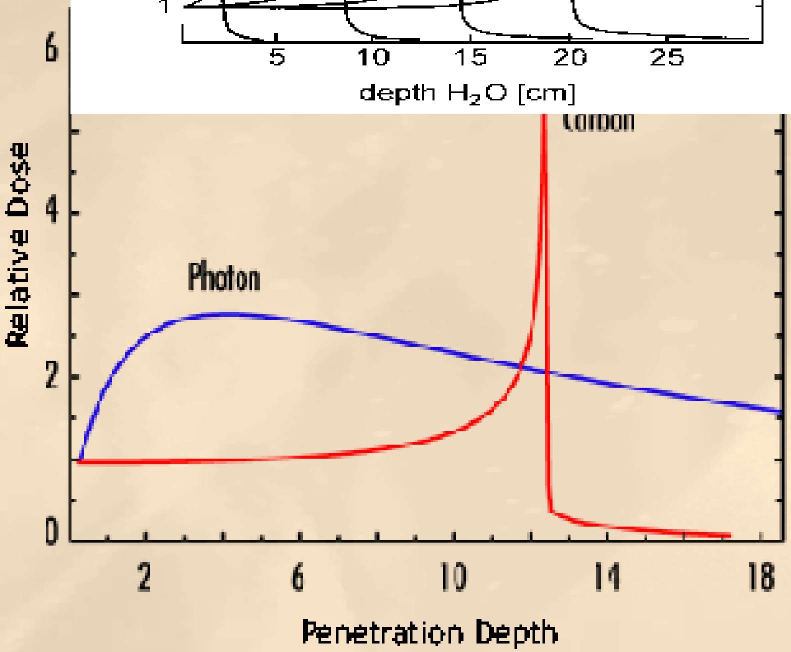
 

4. Origin of human beings, evolution
   of species (to understand it
   from nuclear level)

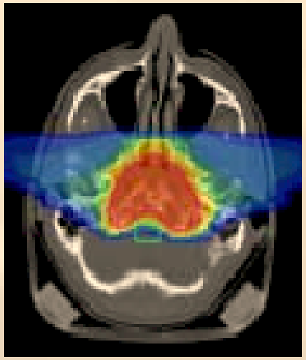
Outline

Cancer Therapy with Ion Beams

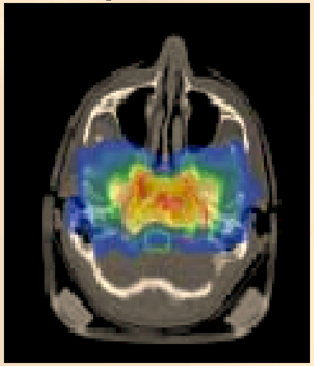




Patient treatment plan

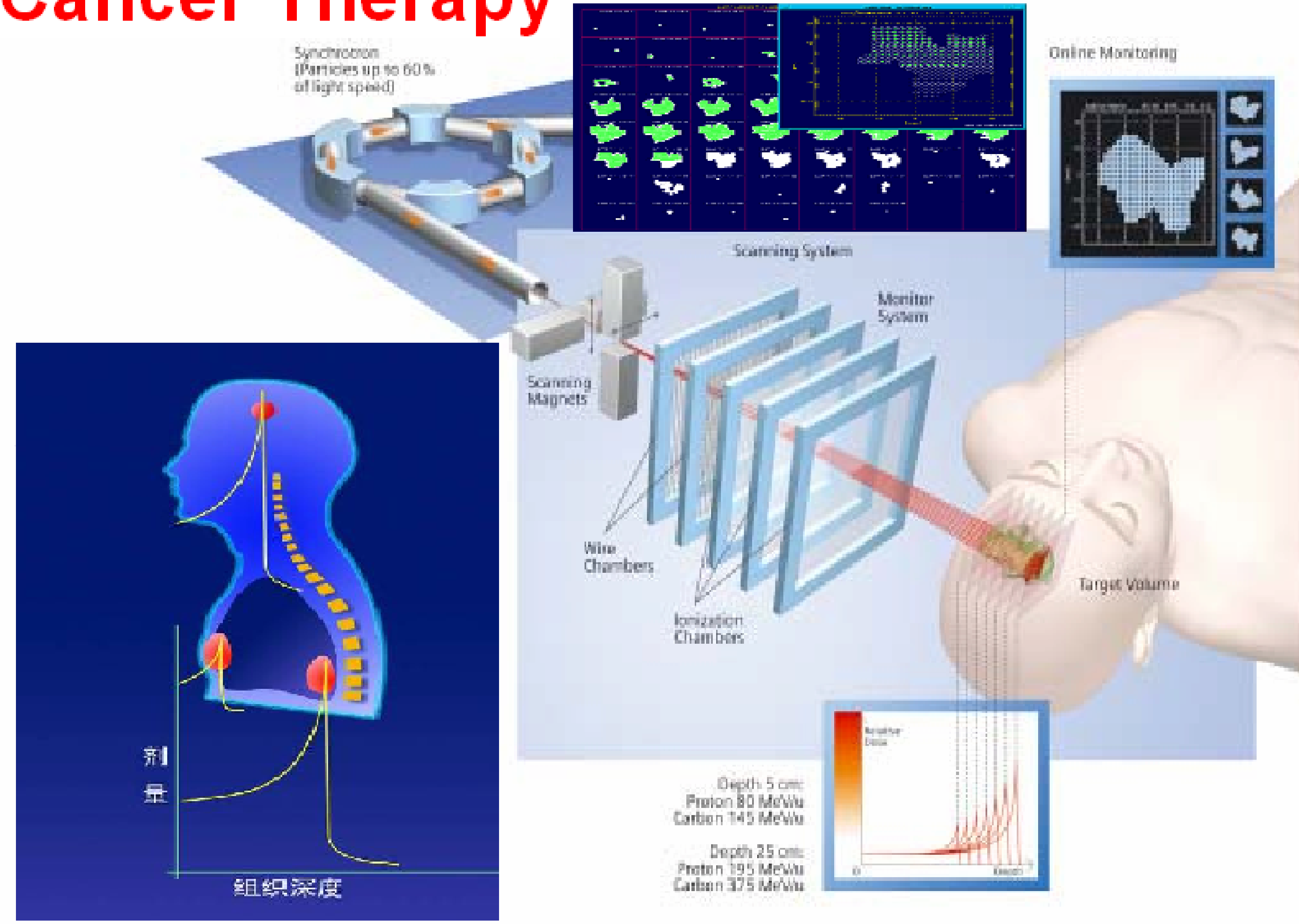


Verification by PET

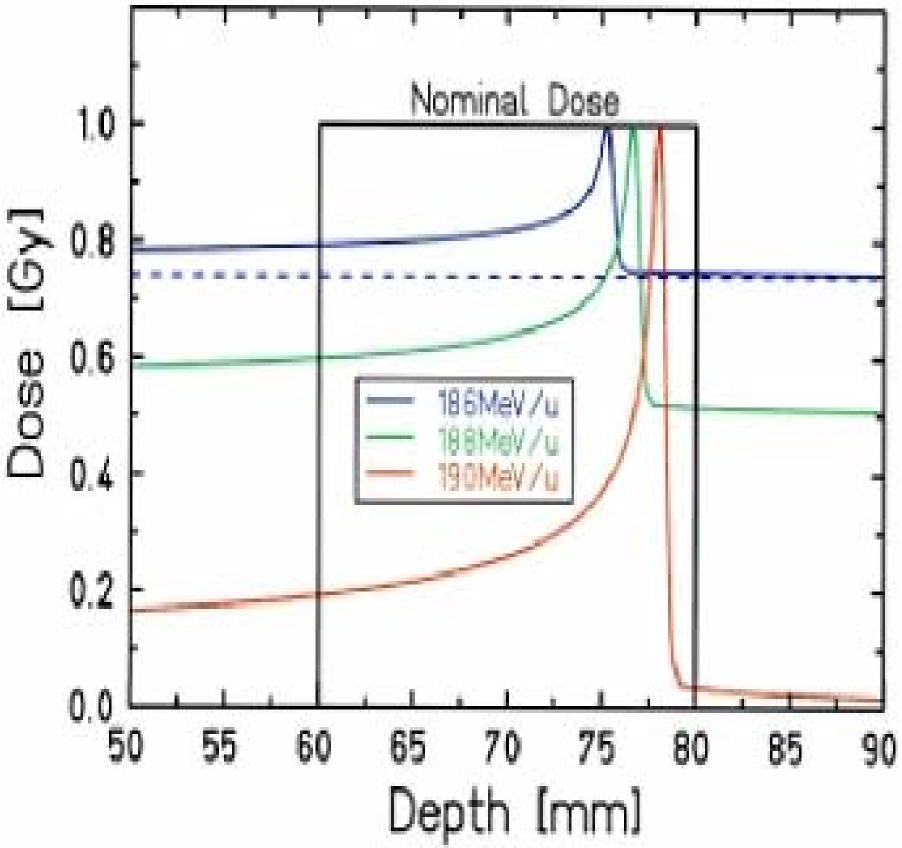


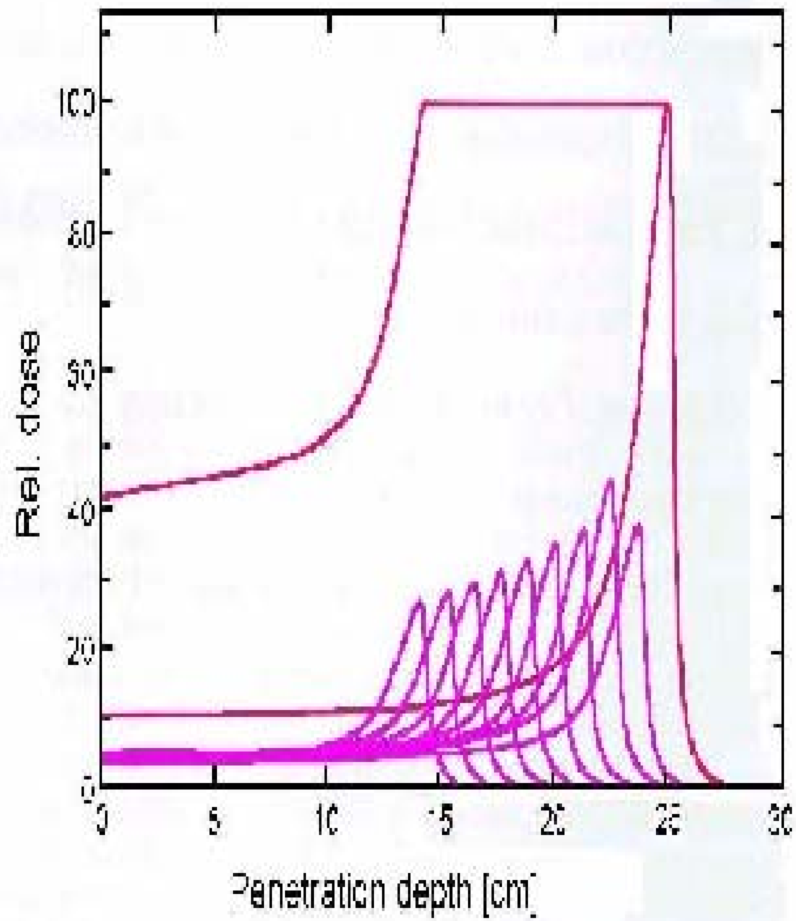
- **67 patients (2200 irradiations)**
- **no side effects**
- **no reoccurence in treated volume**

Cancer Therapy

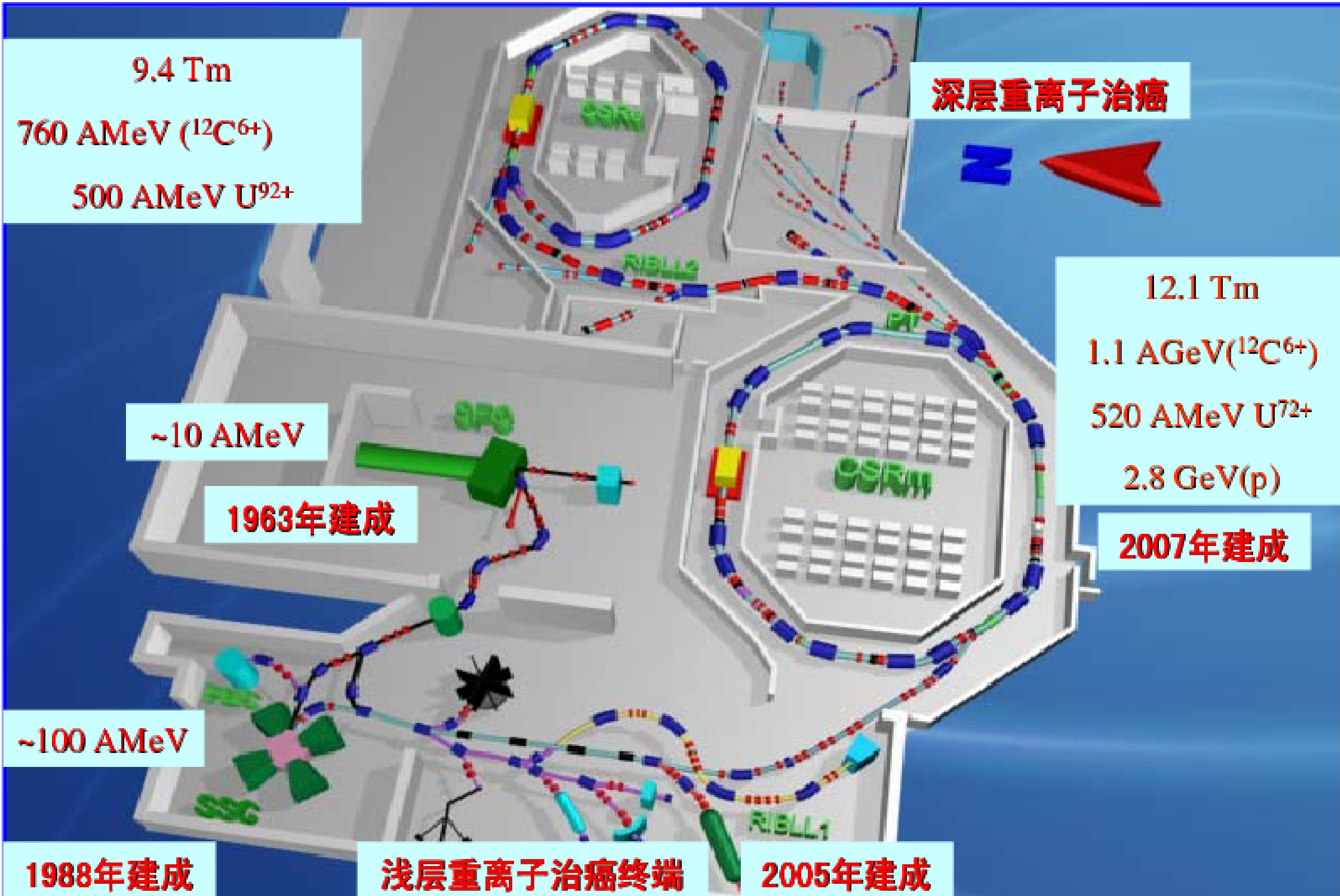


Cancer Therapy





HIRFL-CSR



9.4 Tm
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12C5+イオン照射・花色花型変異

カーネーション
原品種「ビタル」

花色変異：桃
花型変異：丸弁

花色変異：赤
花型変異：丸弁

花色変異：複色（覆輪）
花型変異：丸弁

花色変異：条斑（ストライプ）

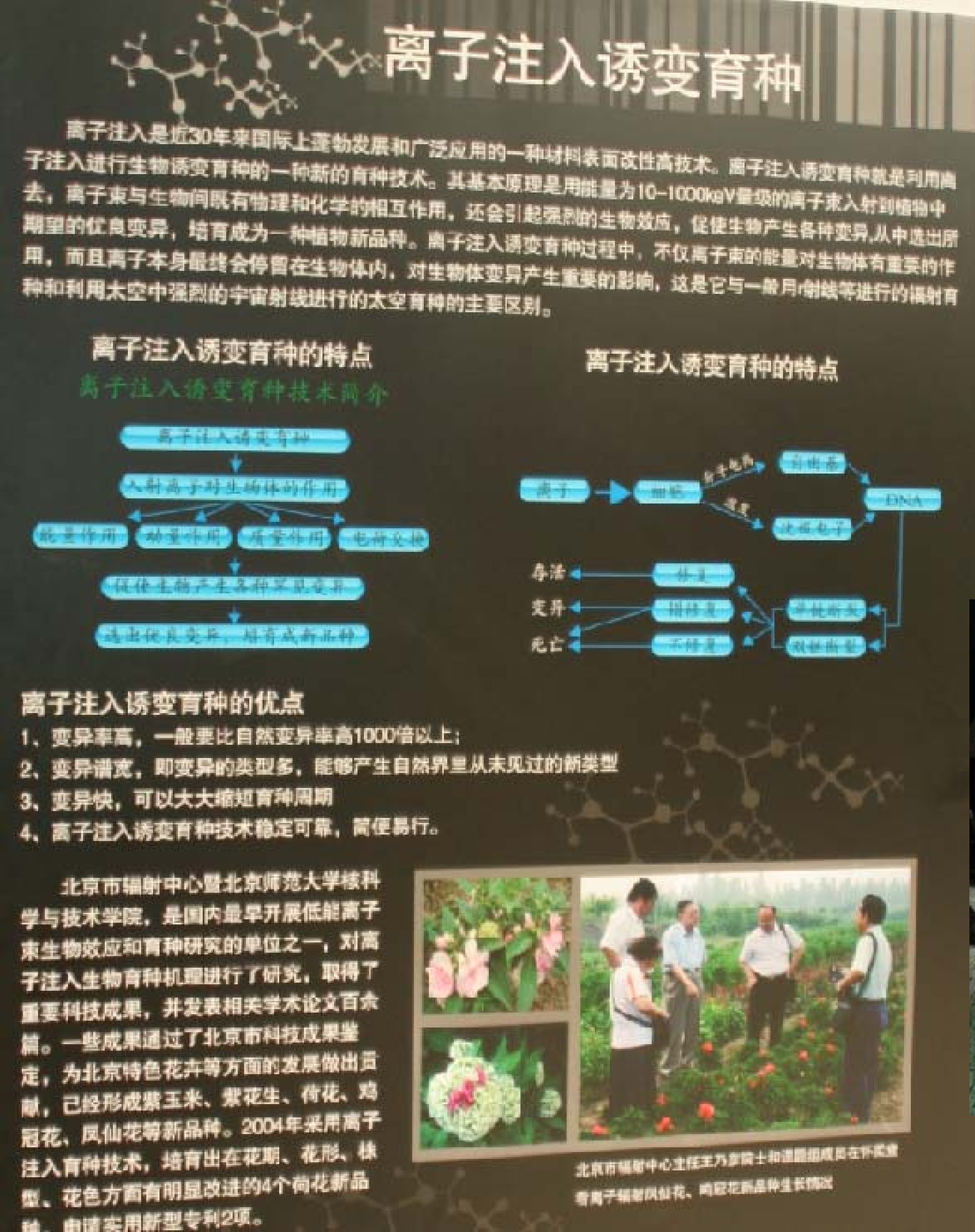
花型変異：ナデシコ弁

キリンビール植物開発研究所
日本原子力研究所高崎研究所

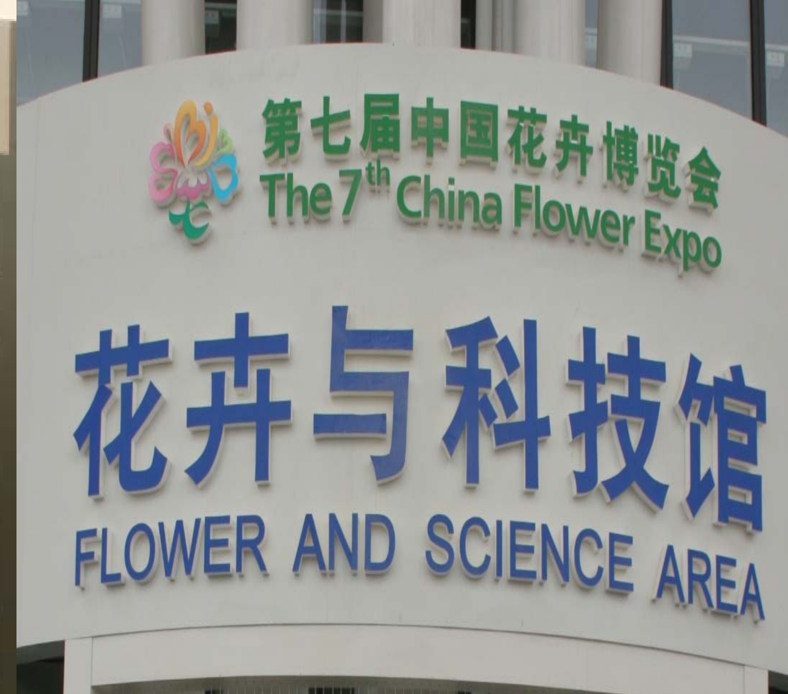
$^{12}C^{5+}$ implantation to the sends of pink

Beijing Normal University, flowers (Balsamine)

对照	中国凤仙1号“春霞”（辐射变异：粉色）	中国凤仙2号“朝阳”（辐射变异：红色）
		
		



离子注入诱变育种
离子注入是近30年来国际上蓬勃发展和广泛应用的一种材料表面改性高技术。离子注入诱变育种就是利用离
子注入进行生物诱变育种的一种新的育种技术。其基本原理是用能量为10-1000keV量级的离子束入射到植物中
去，离子束与生物间既有物理和化学的相互作用，还会引起强烈的生物效应，促使生物产生各种变异,从中选出所
期望的优良变异，培育成为一种植物新品种。离子注入诱变育种过程中，不仅离子束的能量对生物体有重要的作
用，而且离子本身最终会停留在生物体内，对生物体变异产生重要的影响，这是它与一般用射线等进行的辐射育
种和利用太空中强烈的宇宙射线进行的太空育种的主要区别。
离子注入诱变育种的特点
离子注入诱变育种技术简介
离子注入诱变育种
入射离子对生物体的作用
能量作用
动量作用
质量作用
电荷交换
选出优良变异，培育成新品种
离子注入诱变育种的特点
离子
细胞
DNA
存活
变异
死亡
离子注入诱变育种的优点
1、变异率高，一般要比自然变异率高1000倍以上；
2、变异谱宽，即变异的类型多，能够产生自然界里从未见过的新类型
3、变异快，可以大大缩短育种周期
4、离子注入诱变育种技术稳定可靠，简便易行。
北京市辐射中心暨北京师范大学核科
学与技术学院，是国内最早开展低能离子
束生物效应和育种研究的单位之一，对离
子注入生物育种机理进行了研究，取得了
重要科技成果，并发表相关学术论文百余
篇。一些成果通过了北京市科技成果鉴
定，为北京特色花卉等方面的发展做出贡
献，已经形成紫玉米、紫花生、荷花、鸡
冠花、凤仙花等新品种。2004年采用离子
注入育种技术，培育出在花期、花形、株
型、花色方面有明显改进的4个荷花新品
种，申请实用新型专利2项。



第七届中国花卉博览会
The 7th China Flower Expo
花卉与科技馆
FLOWER AND SCIENCE AREA

证书
证书
证书
证书

奖章、奖杯

（10） 其它进展

cockscombs (after radiations)









27 3:13PM





Beijing Lotus Flower Park (collaboration)

园林动态 PARK DYNAMIC

工作动态

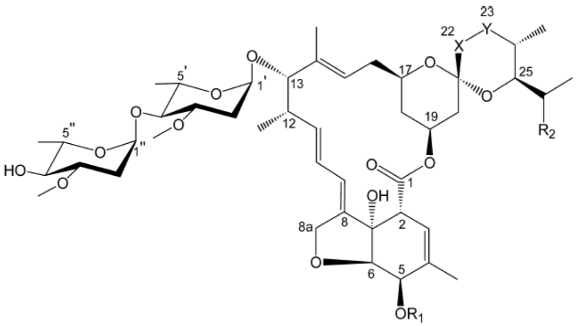
第九届北京莲花池荷花节盛大开幕

6/24/2009 17:10:37 莲花池公园 李雅丽

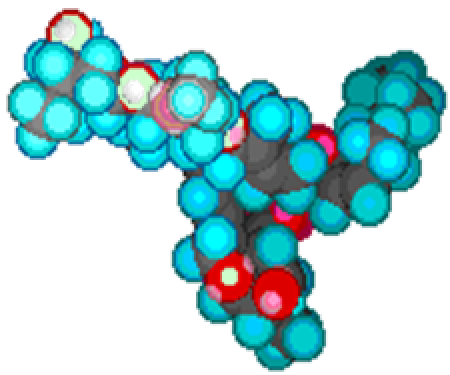
第九届北京莲花池荷花节于6月24日上午在莲花池公园东广场表演舞台举行了隆重的开幕仪式。原全国人大常委会副委员长何鲁丽、北京师范大学核科学与技术学院副院长张丰收、北京市园林绿化局科技处处长徐佳、北京市公园管理中心处长王鹏训、北京市园林绿化局公园林场风景名胜处副处长张亚红、太平桥街道工委书记郗俊生、办事处主任何秋香、丰台区园林局局长申燕民、局长助理程朝晖等嘉宾出席了开幕仪式。

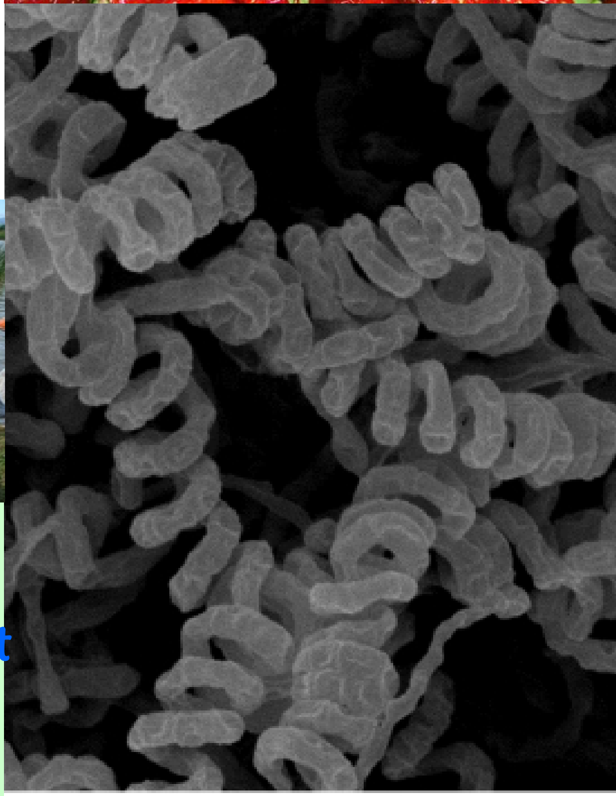
Lotus Seeds get larger

Green pesticide (Avermitilis, Spinosad)



	R1	R2	X-Y
Avermectin A1a	CH_3	C_2H_5	CH=CH
A1b	CH_3	CH_3	CH=CH
A2a	CH_3	C_2H_5	CH_2-CH(OH)
A2b	CH_3	CH_3	CH_2-CH(OH)
B1a	H	C_2H_5	CH=CH
B1b	H	CH_3	CH=CH
B2a	H	C_2H_5	CH_2-CH(OH)
B2b	H	CH_3	CH_2-CH(OH)



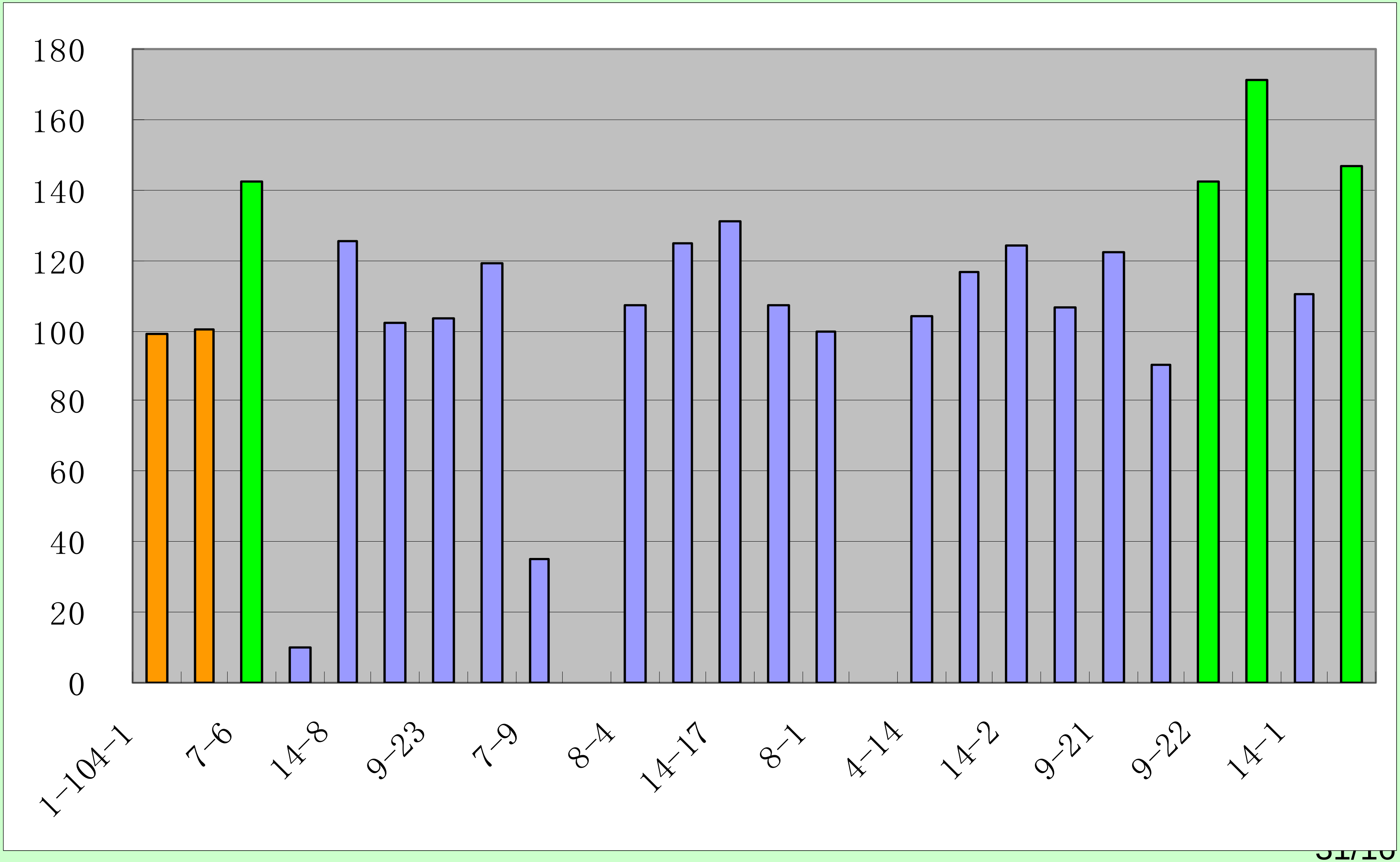


Streptomyces avermitilis **sp. nov.**
Int J. Syst Evol. Microbiol. **52**: 2011-2014 (2002)

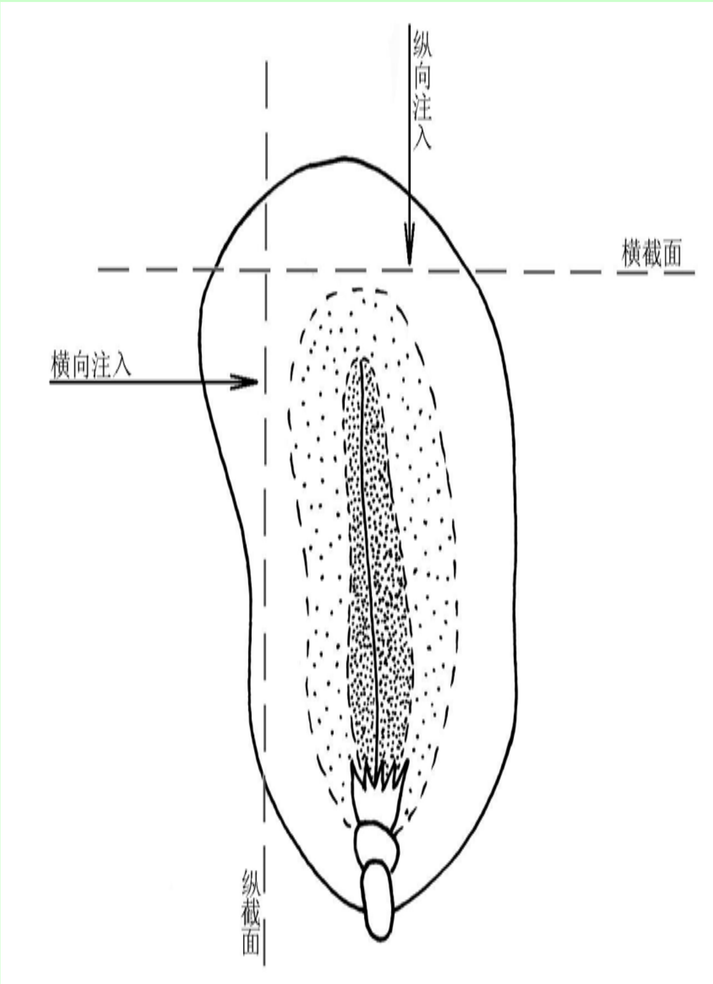
- Very low leave behind, easy decomposition with Sunlight, friendly for health and environment
- The price is high !

Prelimimary results –Spinosad-

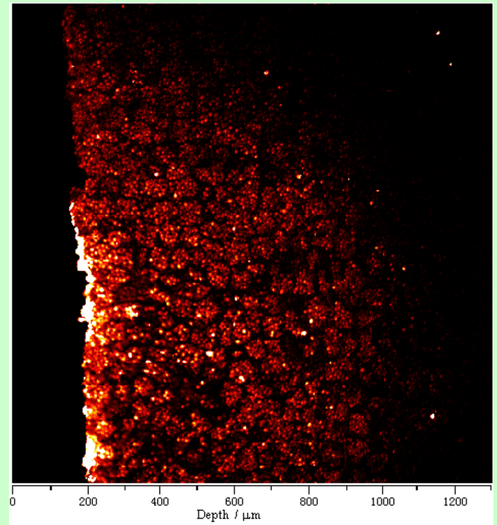
(collaboration with the Institute of Microbiology, CAS)

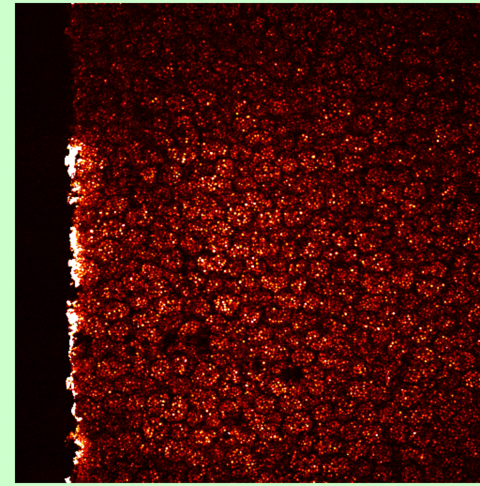


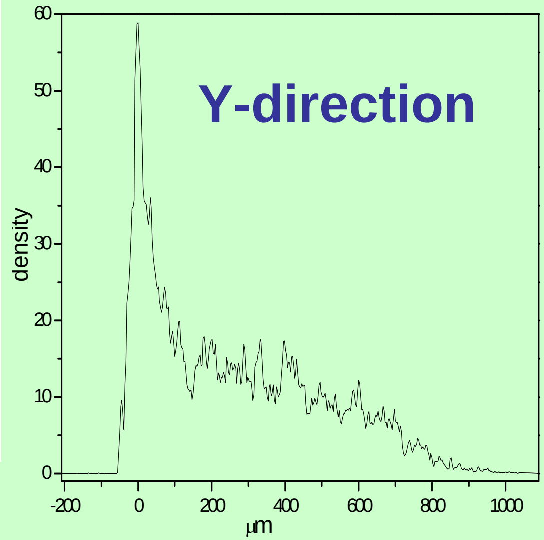
peanut

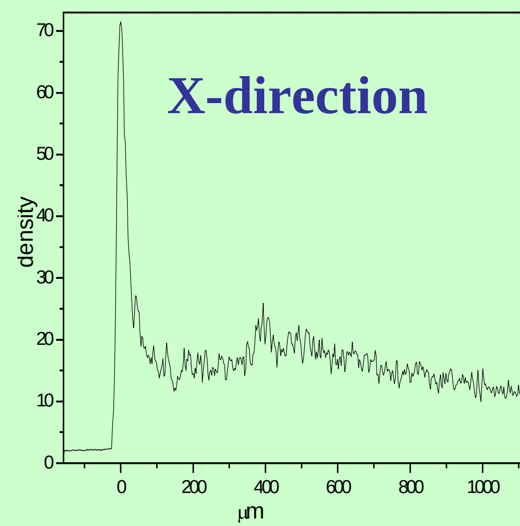


Profile of peanut seed









Vanadium^{+}(9x10^{16}/cm^{2}) at 200keV, Concentration-d, (TPLSM method)

Outline

1. Introduction

2. Applications

    2.1 Cancer therapy

    2.2 Seed breeding

    2.3 Space radiation

    2.4 Problems

3. A Multi-scale microscopic dynamical model

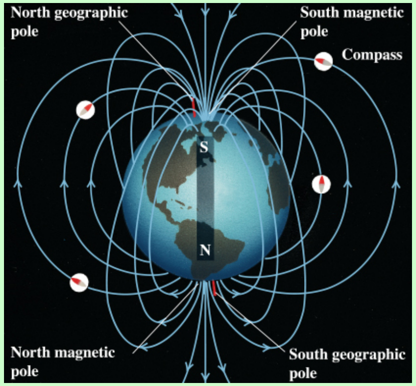
4. Conclusions

Three kinds of space radiations

Cosmic Rays

solar protons

high energy electrons and protons trapped by the Earth's magnetic field.



Chinese academy of agriculture：space seed breeding

南瓜身形如钟(Pumpkin)

彩棉是纯天然(Cotton)

太空佛手茄子(Eggplant)

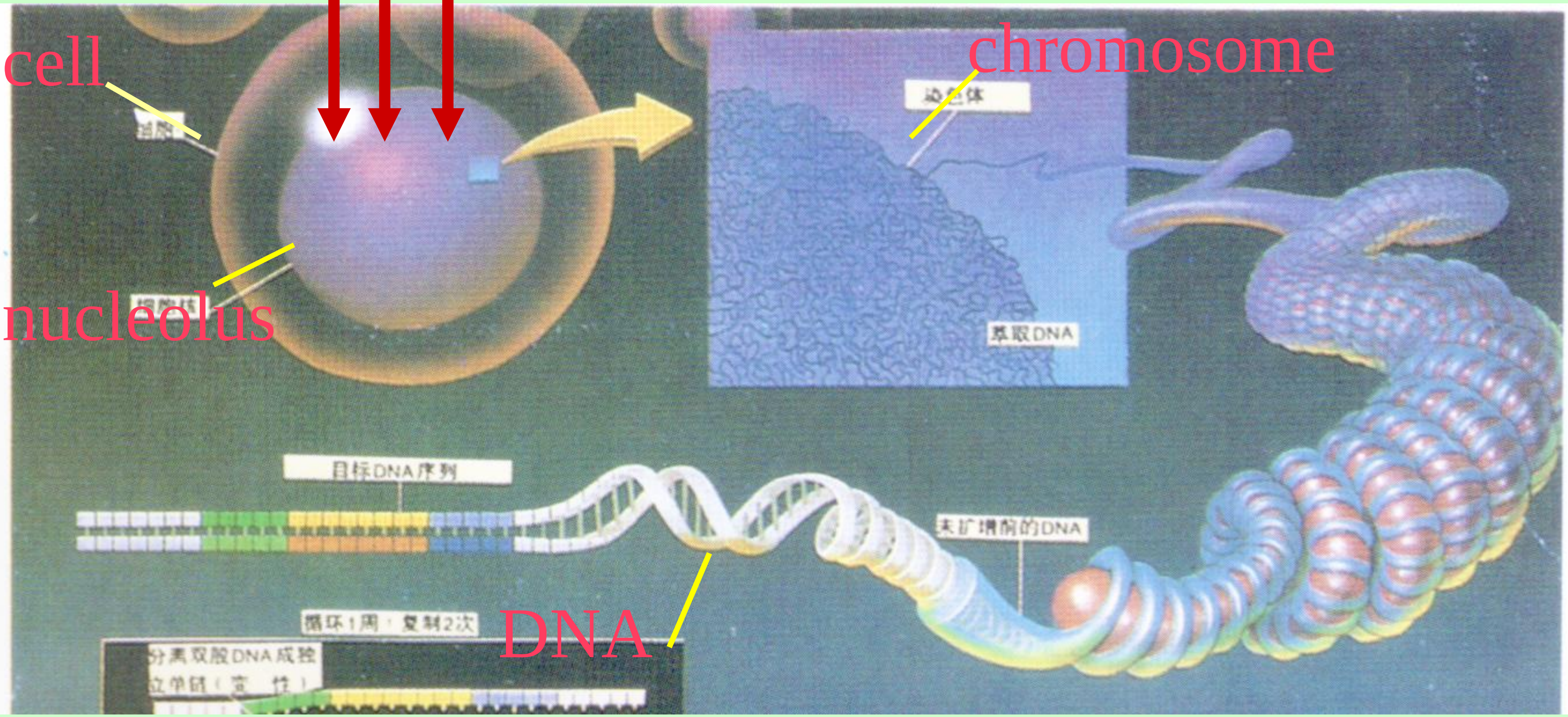
Outline

Common problem: ***heavy ion interactis with biomolecules***

Heavy Ions

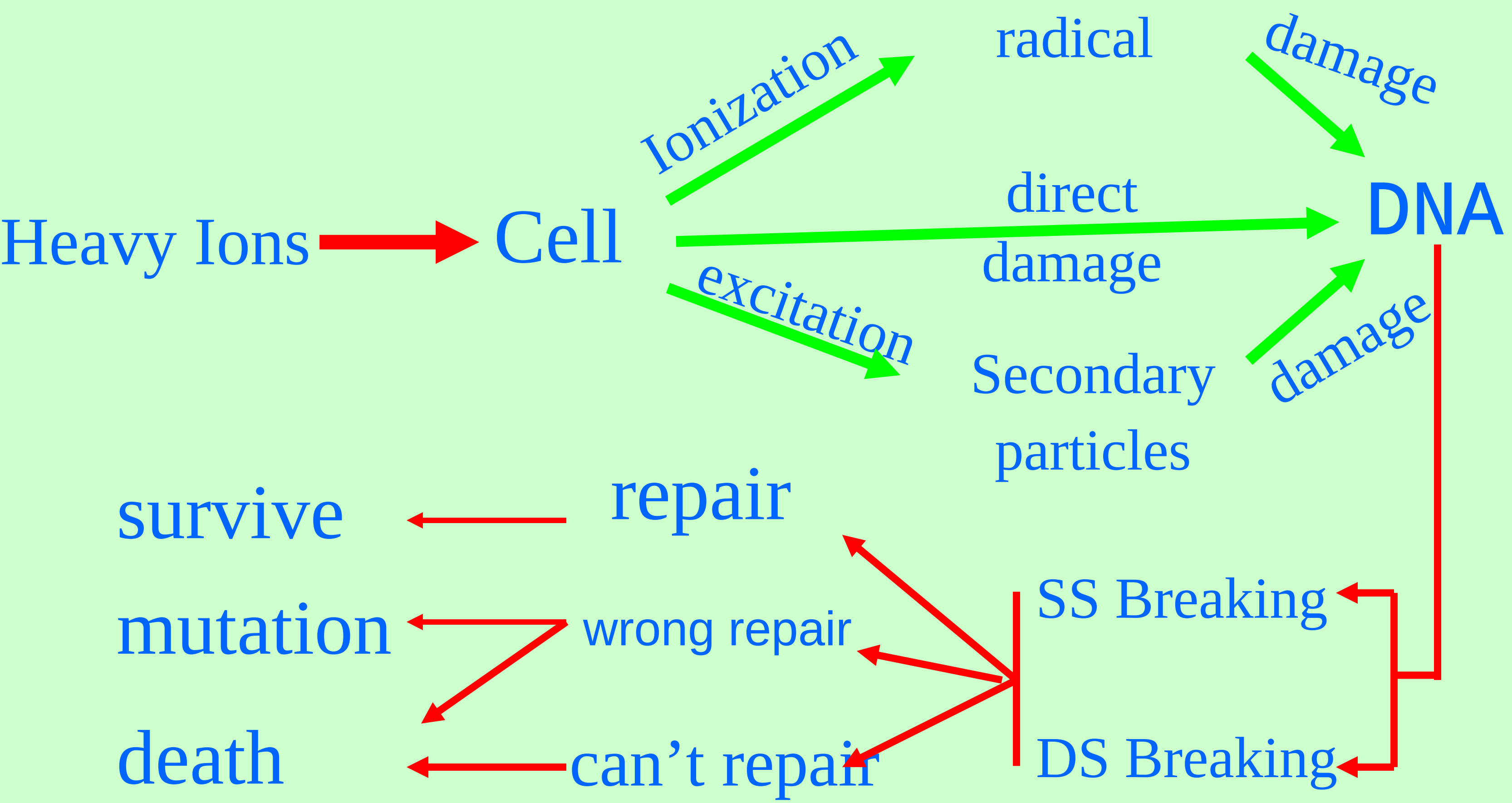
Nuclear Process, Electron excitation

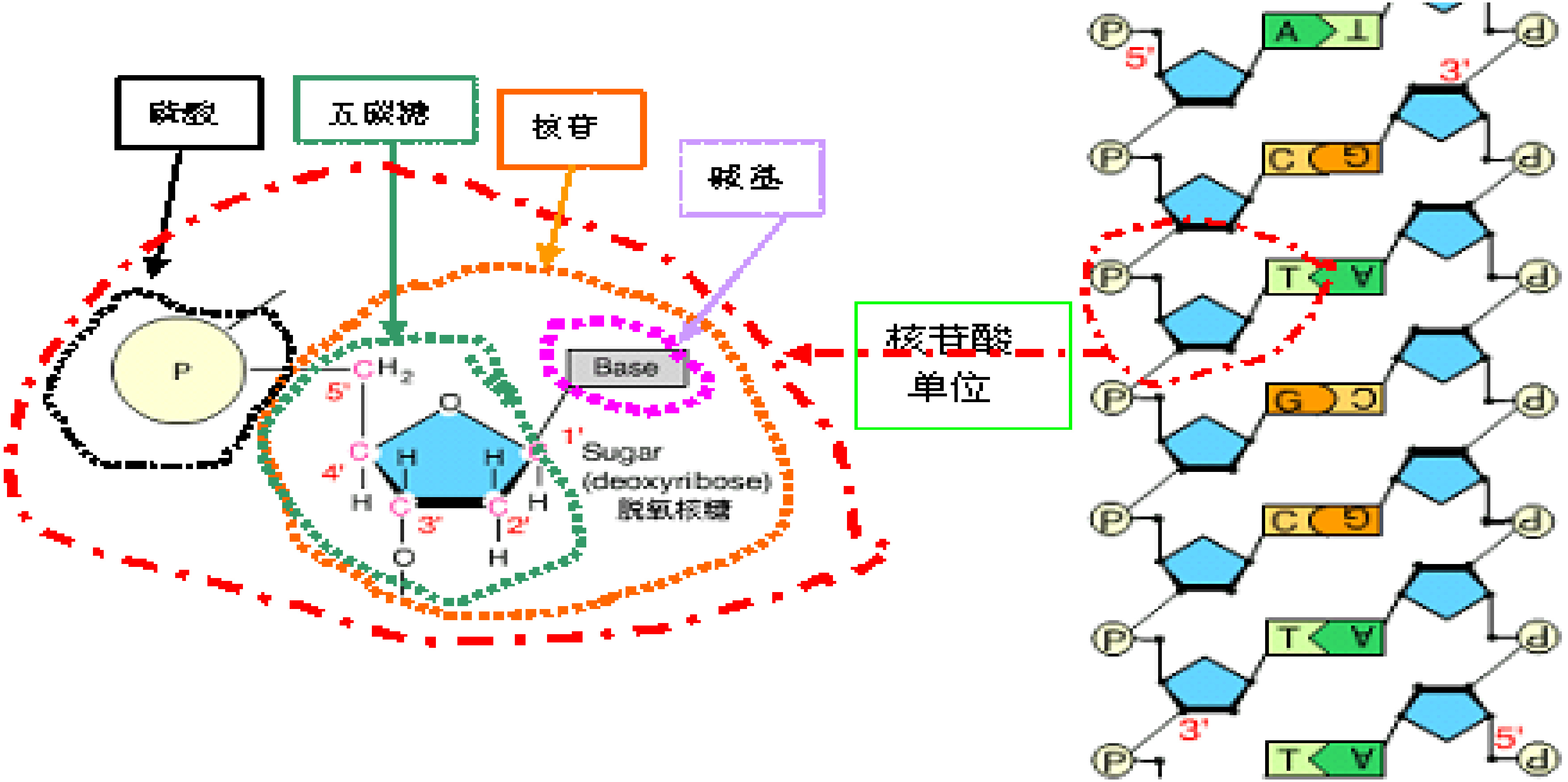
Relaxation, to a new structure

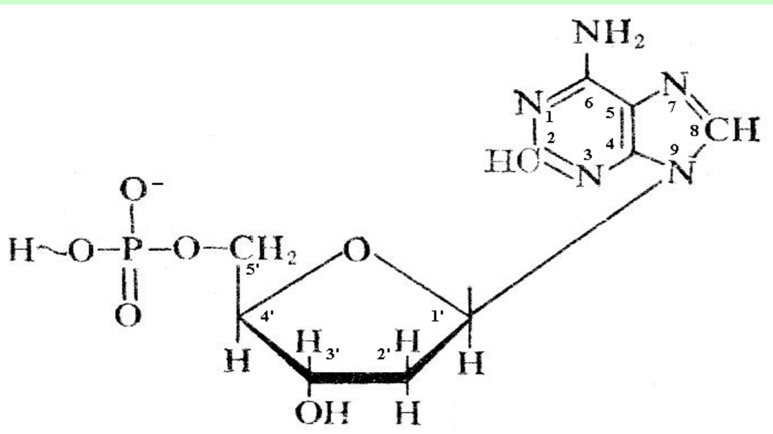


Cell, nucleolus, chromosome, DNA

mutation mechanism

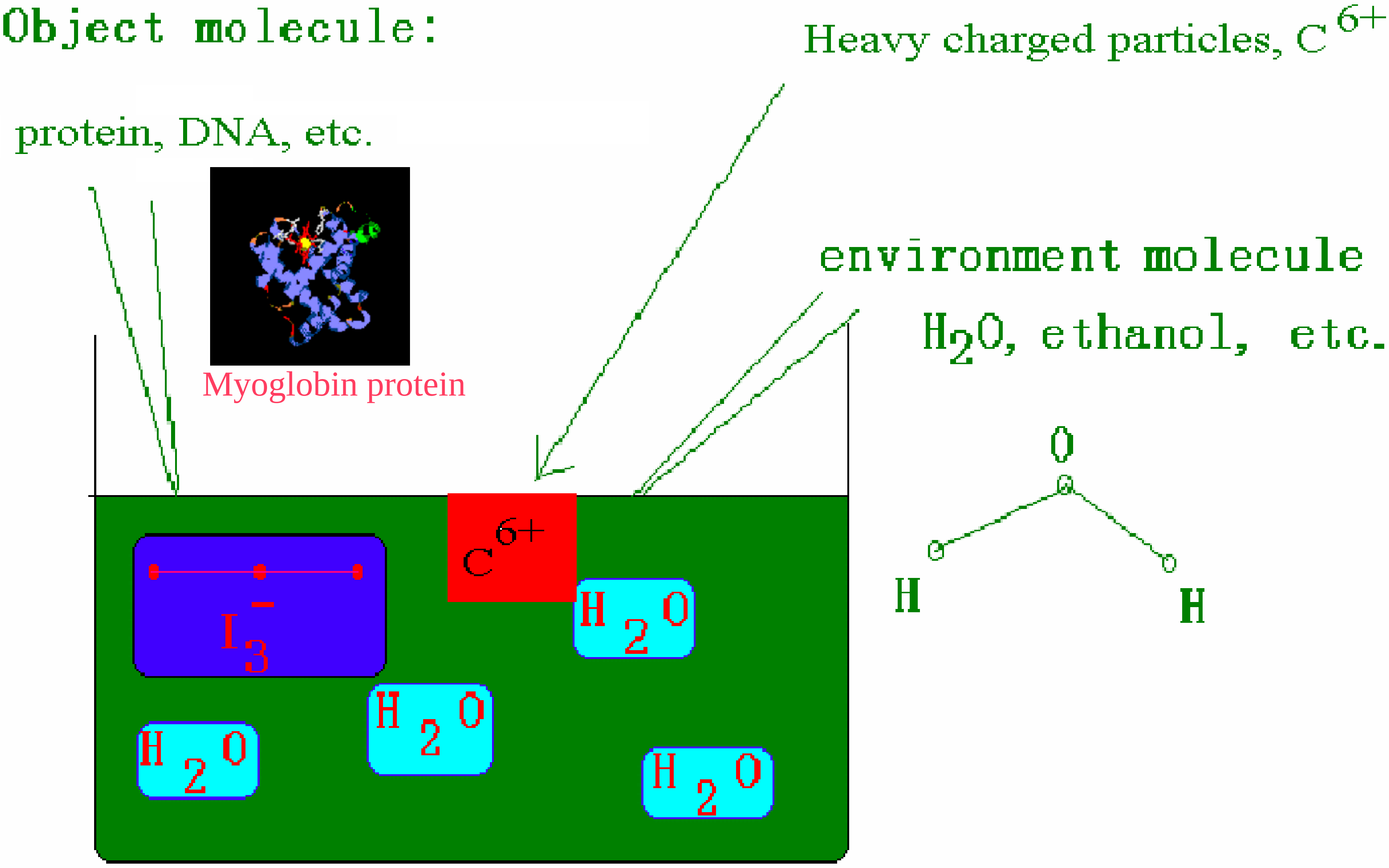



五碳糖
核苷
碱基
核苷酸单位
Base
Sugar
(deoxyribose)
脱氧核糖




SSB
DSB

Experiments: biological molecule therapy with heavy charged particles



Physics analysis

- Object (Solute, protein,DNA, etc)
- solvent molecules (water, etc.)
- incident particles (heavy charged particles, x-rays, photons)

☺Physical process: *projectile fragmentation*, ionization,electron transport and emission, linear energy loss, strong potential energy and polarization, internal structure changes, etc.

Outline

1. Introduction

2. Applications

 2.1 Cancer therapy

 2.2 Seed breeding

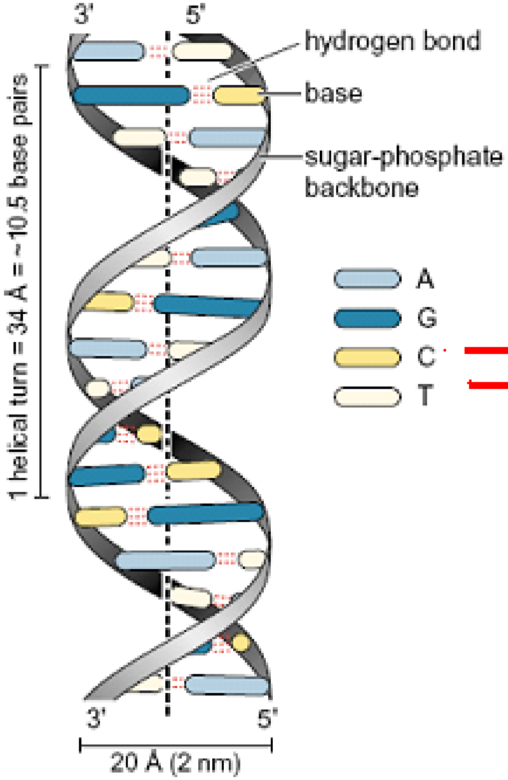
 2.3 Space radiation

 2.4 Problems

3. A Multi-scale microscopic dynamical model

4. Conclusions

A multi-scale microscopic dynamic approach to study interaction of heavy ions with biomolecules



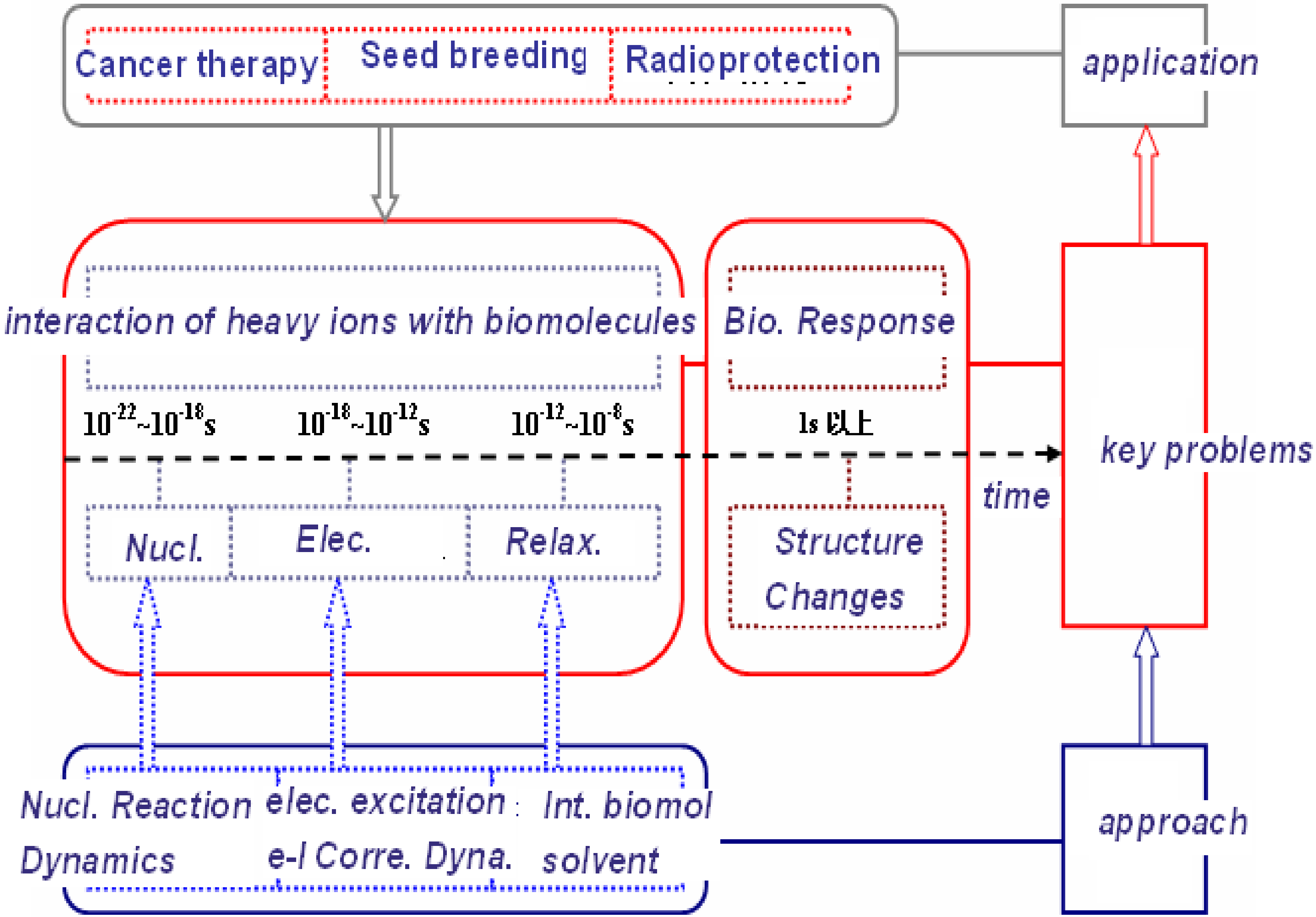
⇒ **New Structure !**

⇓

⇓ Physical process(10^{-24}~10^{-8}s) ⇒ ⇓ Chemical process(10^{-8}s) ⇒ ⇓ Biological process (10^{3}s)

⇓

⇓ Nuclear process (10^{-24}~10^{-18}s) ⇒ ⇓ Electronic process (10^{-18}~10^{-12}s) ⇒ ⇓ Relaxation process (10^{-12}~10^{-8}s)



Cancer therapy
Seed breeding
Radioprotection
application
interaction of heavy ions with biomolecules
Bio. Response
10^{-22}~10^{-18}s
10^{-18}~10^{-12}s
10^{-12}~10^{-8}s
1s 以上
key problems
time
Nucl.
Elec.
Relax.
Structure
Changes
Nucl. Reaction
Dynamics
elec. excitation
e-I Corre. Dyna.
Int. biomol
solvent
approach

Decomposition of this approach

(1). Nuclear multifragmentation (C, N, and Ne induced reactions)

(2). Electrons excitations during interactions of beam and/or fragments with molecules

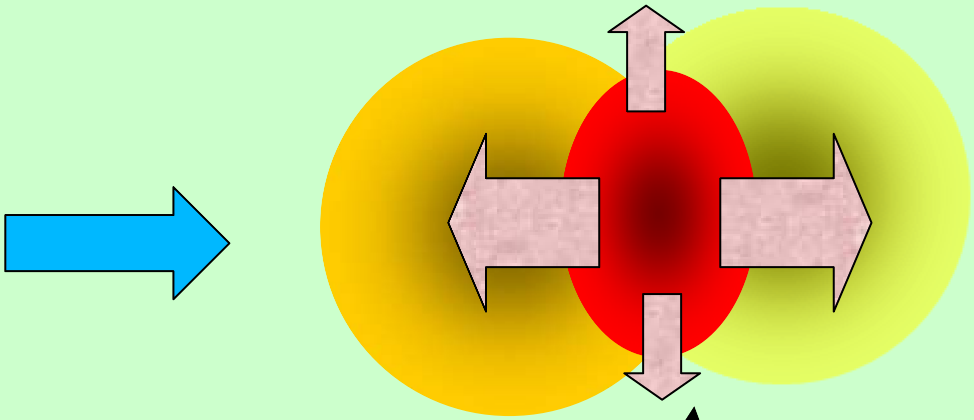
(3). Dose distributions

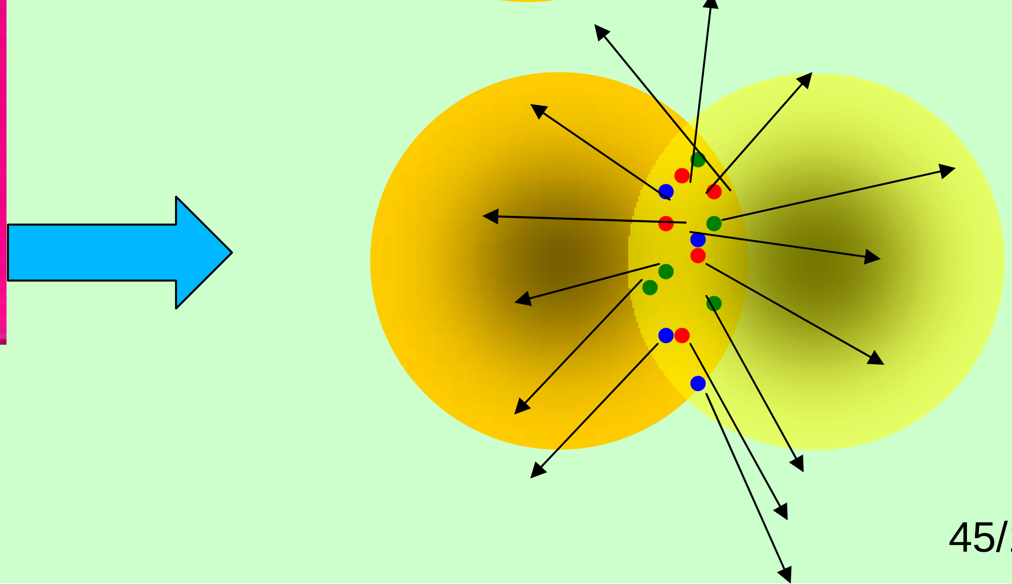
(4). Properties of sub-unit of DNA, such as adenine(A), thymine(T), C,G,U

(5). Structure changes of DNA

(6). Structure-->biological functions ?

(1)Nuclear Multifragmentation





Nuclear Multifragmentation，
F. S. Zhang and L. X. Ge,
Science Press, Beijing, 1998

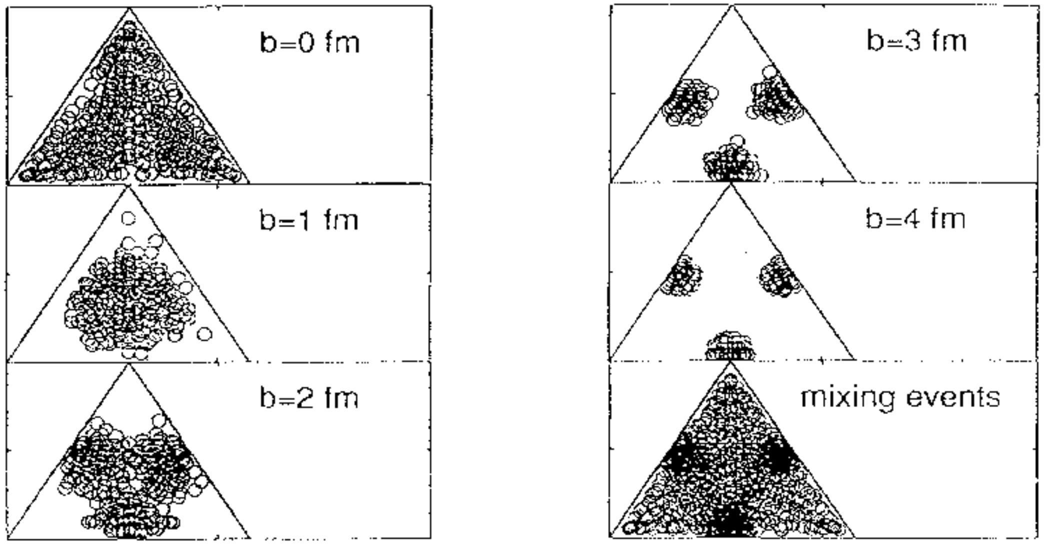


FIG. 8. The correlations between the three largest fragments of an event by a charge-Dalitz plot for the $^{40}Ca+^{40}Ca$ system at 90 MeV/nucleon with the events of impact parameters 0, 1, 2, 3, 4 fm and the mixing events with different impact parameters except $b = 0$ fm. The number of events is the same as in Fig. 5.

Zhang and Suraud,

Phys. Rev. C51,1995,3201

$^{40}Ca+^{40}Ca$, 90 MeV/u

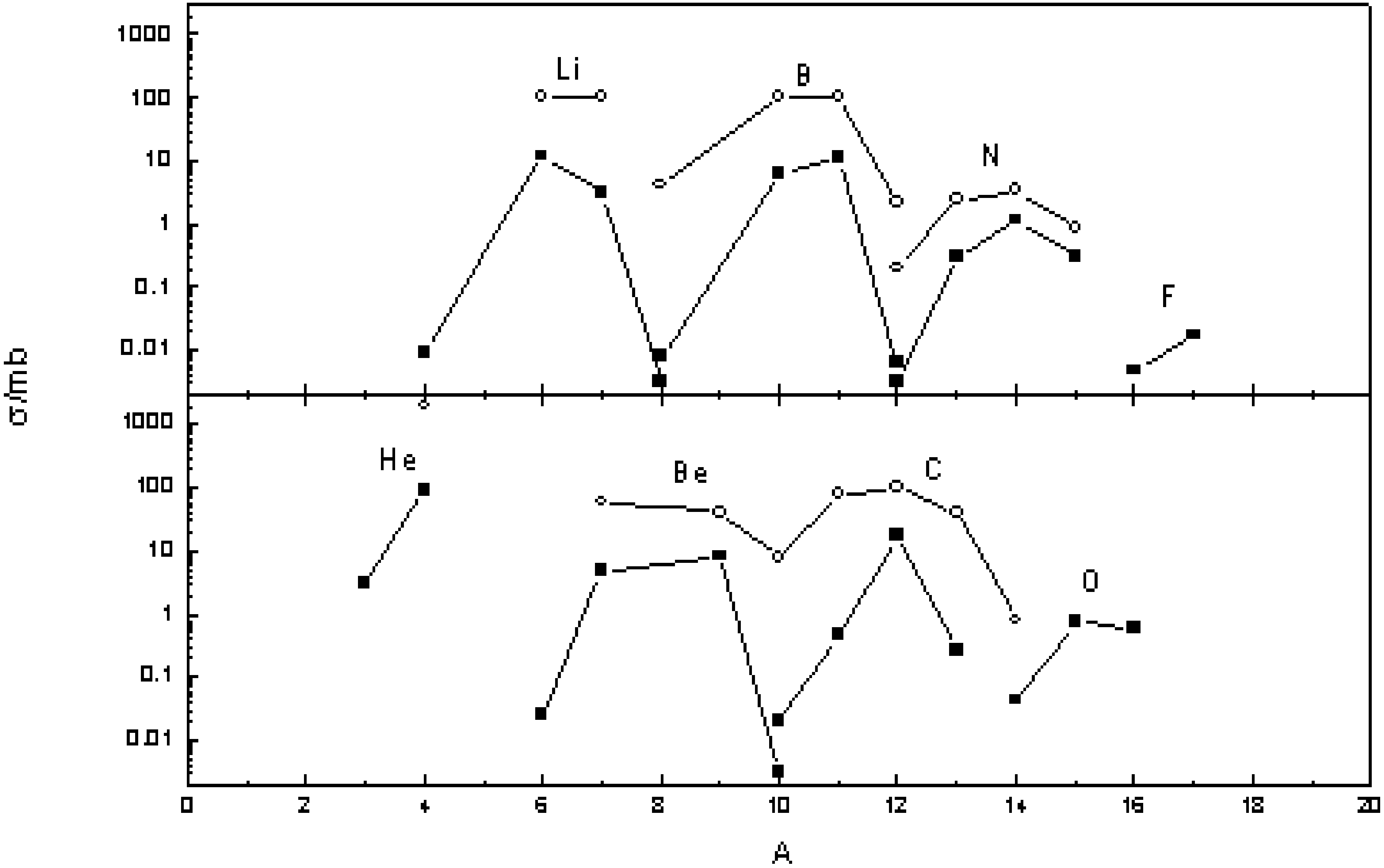
$\sigma_{tot} \approx 1.5 \times 10^{-24}\ cm^2$

$\sigma_{frag} \approx 1.2 \times 10^{-25}\ cm^2$

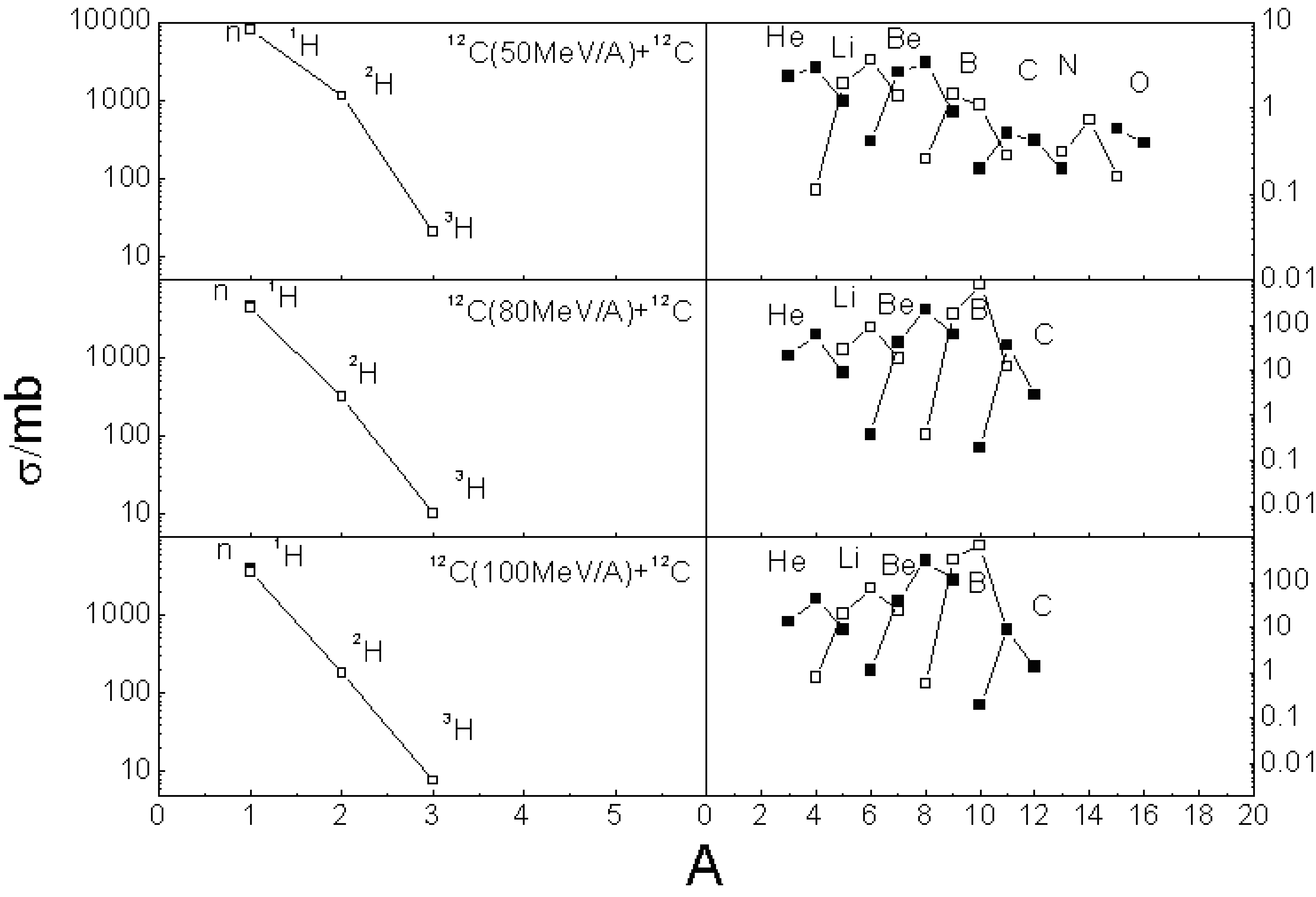
$\sigma_{frag} / \sigma_{tot} \approx 8\ \%$

$^{12}C+^{12}C$, 28.7 MeV/u

Exp. Czudek et al, *Phys. Rev.* C43(1991)1248）

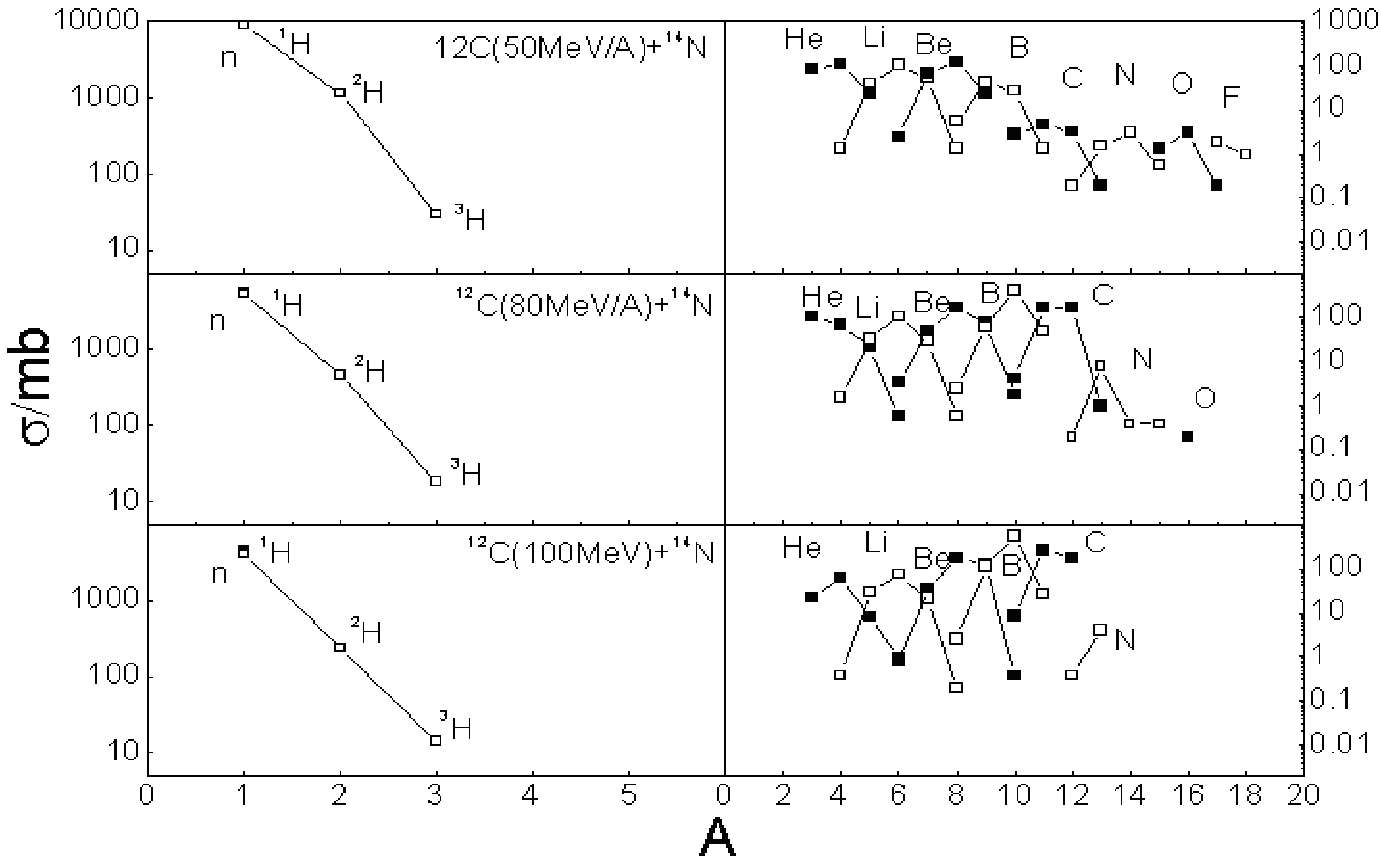


$^{12}C+^{12}C$



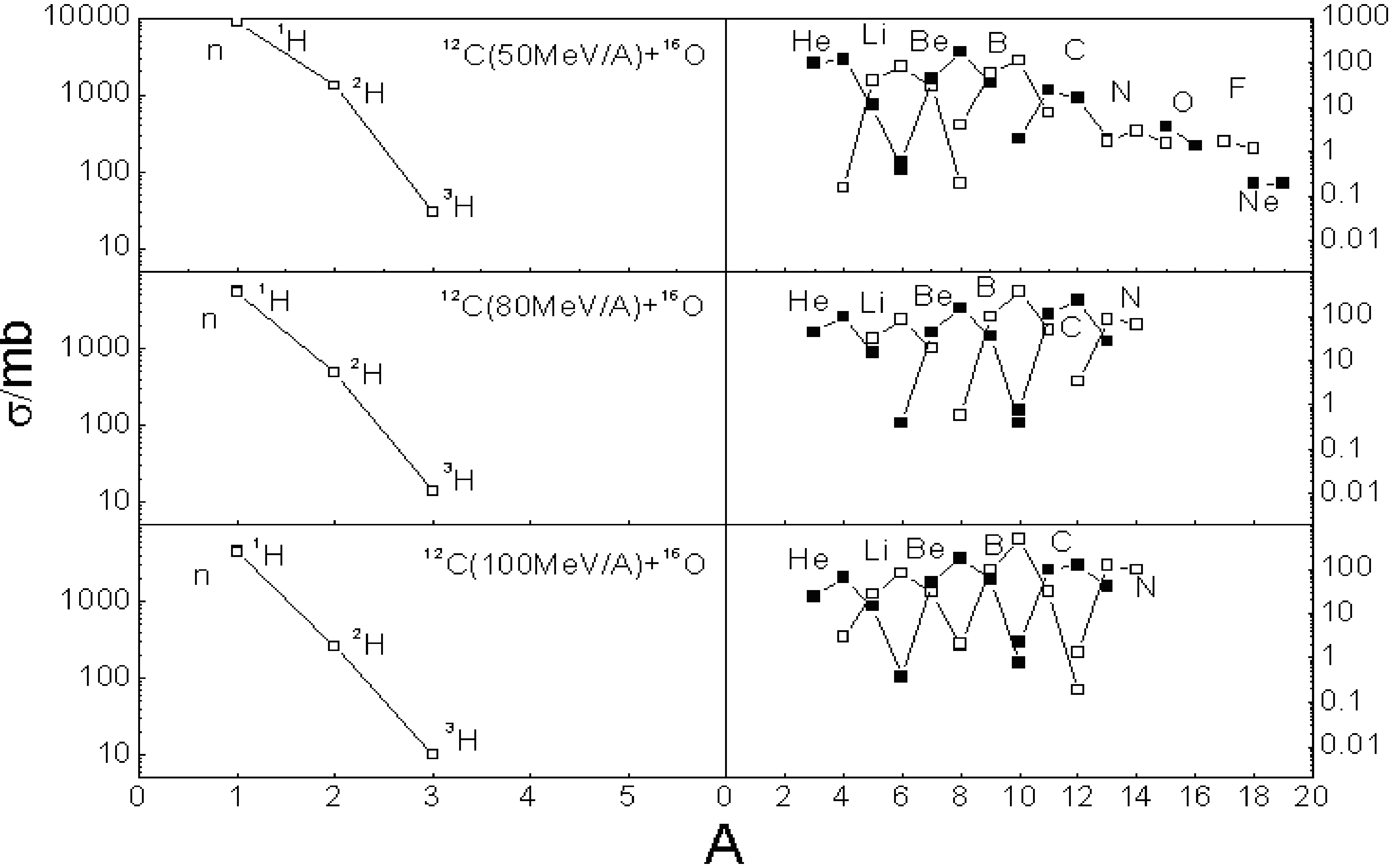
σ/mb
A
n
^{1}H
^{2}H
^{3}H
^{12}C(50MeV/A)+^{12}C
^{12}C(80MeV/A)+^{12}C
^{12}C(100MeV/A)+^{12}C
He
Li
Be
B
C
N
O

$^{12}C+^{14}N$



12C(50MeV/A)+14N
12C(80MeV/A)+14N
12C(100MeV)+14N
n
1H
2H
3H
He
Li
Be
B
C
N
O
F
σ/mb
A

$^{12}C+^{16}O$


12C(50MeV/A)+16O
12C(80MeV/A)+16O
12C(100MeV/A)+16O
n
1H
2H
3H
He
Li
Be
B
C
N
O
F
Ne
σ/mb
A

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Nuclear Physics A 807 (2008) 71–78

NUCLEAR PHYSICS A

www.elsevier.com/locate/nuclphysa

Fragmentation cross sections of ^{20}Ne collisions with different targets at 600 MeV/nucleon

Bao-An Bian [a,b], Feng-Shou Zhang [a,b,c,*], Hong-Yu Zhou [a,b]

[a] *The Key Laboratory of Beam Technology and Material Modification of Ministry of Education, Institute of Low Energy Nuclear Physics, Beijing Normal University, Beijing 100875, China*

[b] *Beijing Radiation Center, Beijing 100875, China*

[c] *Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator of Lanzhou, Lanzhou 730000, China*

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Available online 3 April 2008

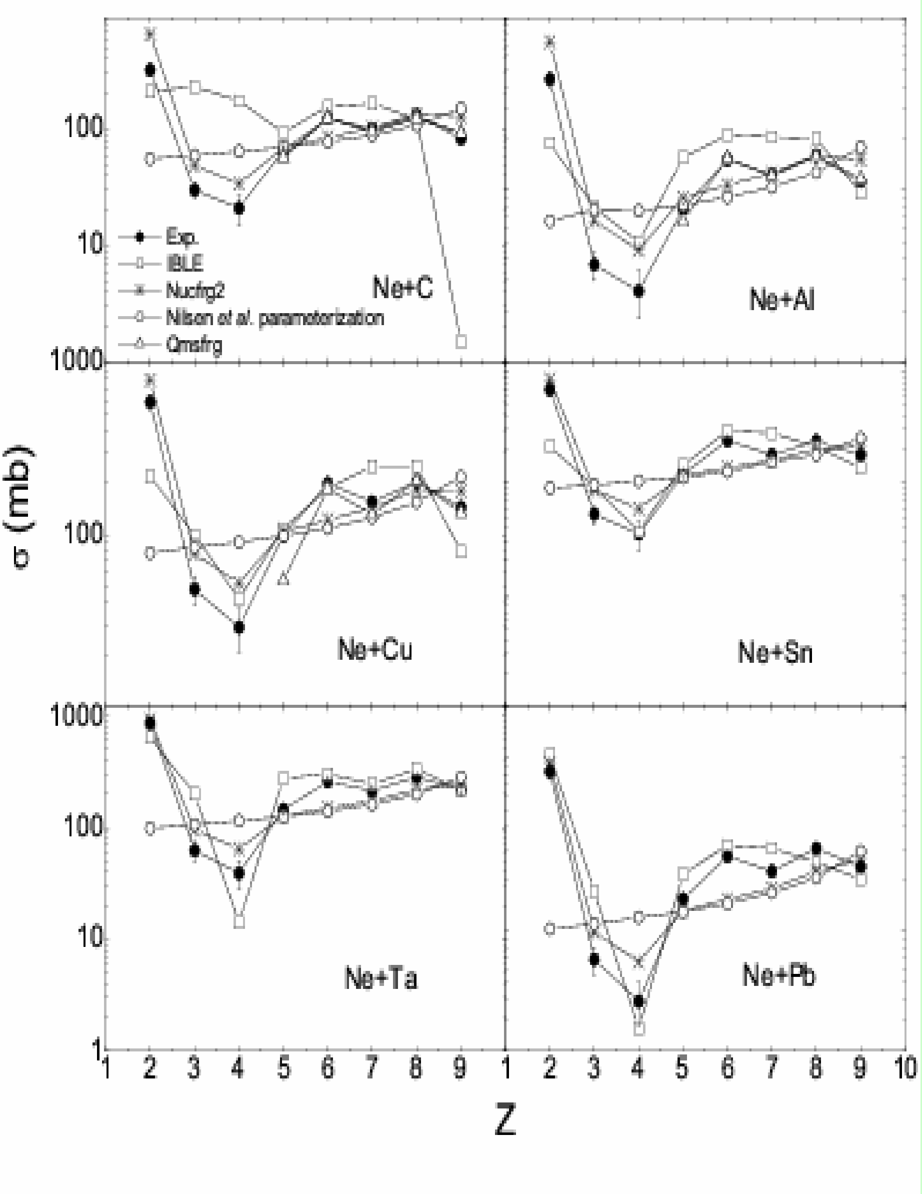
Abstract

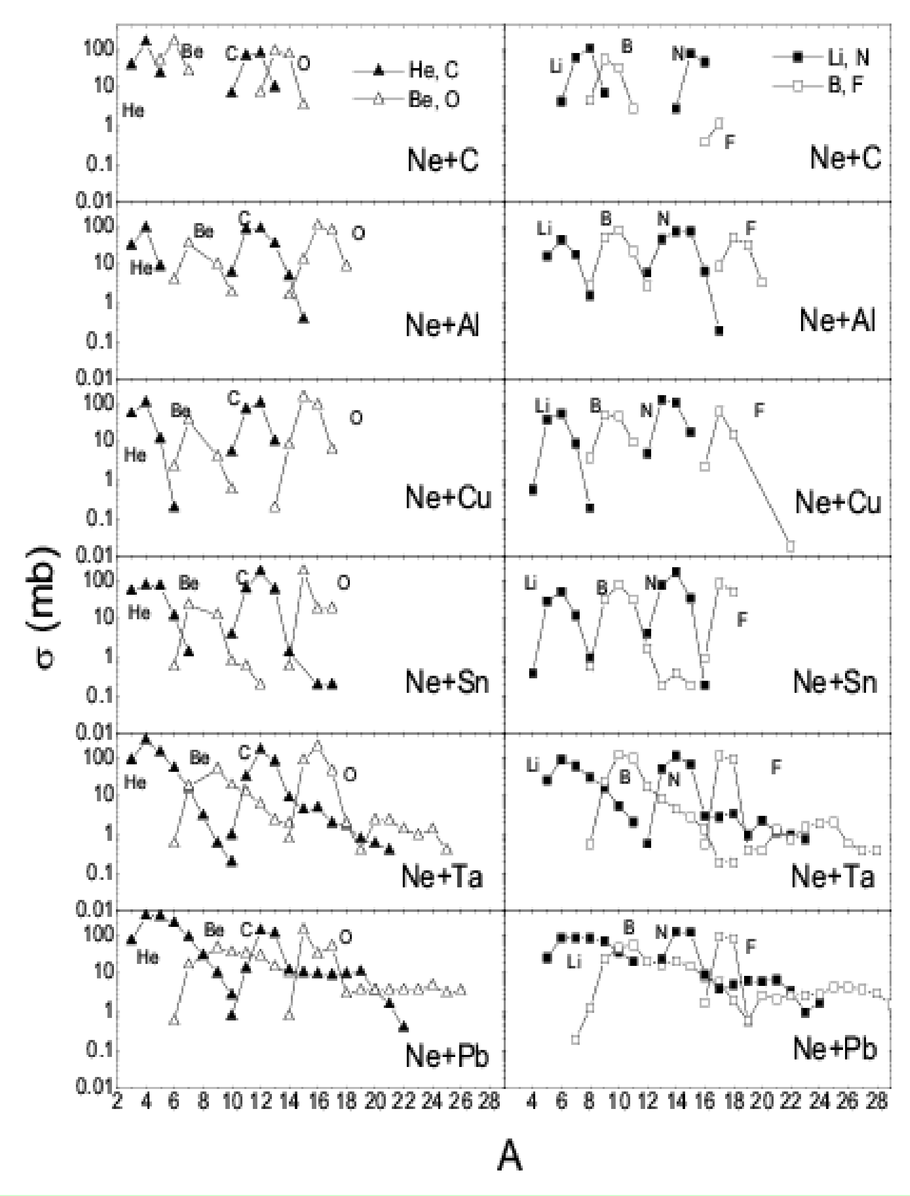
Within the framework of the isospin-dependent Boltzmann–Langevin equation, the production cross sections of fragments are calculated for reactions of Ne collisions with C, Al, Cu, Sn, Ta, and Pb targets at 600 MeV/nucleon. It is found that the production cross sections for fragments $Z = 2$ to 9 are qualitatively reproduced by the present calculations except for C target. The enhancement of even-Z fragments (C, O) cross sections shown in the experimental data is not well reproduced except for Ta target, however the observed suppression of the F fragment cross sections is described very well. The suppression of F production is discussed in terms of isotopic distribution of fragments. This is the first time to use the isospin-dependent Boltzmann–Langevin equation model to calculate the fragmentation cross sections for these reaction systems.

PACS: 25.70.-z; 25.70.Pq; 98.70.Sa

Keywords: Low and intermediate energy heavy-ion reactions; Multifragment emission; Cosmic rays

Isotope distributions





PHYSICAL REVIEW C **83**, 014608 (2011)

Odd-even effect in heavy-ion collisions at intermediate energies

Jun Su,[1,2] Feng-Shou Zhang,[1,2,3,*] and Bao-An Bian[4]

[1] *College of Nuclear Science and Technology, Beijing Normal University, 100875 Beijing, China*
[2] *Beijing Radiation Center, Beijing 100875, China*
[3] *Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator of Lanzhou, Lanzhou 730000, China*
[4] *School of Science, Jiangnan University, Wuxi, Jiangsu 214122, China*

(Received 7 December 2010; published 31 January 2011)

Heavy-ion collisions at intermediate energies are studied by the isospin-dependent quantum molecular dynamics model in the company of the GEMINI model. The isospin-dependent quantum molecular dynamics model is applied to describe the violent stage of the collisions, while the GEMINI model is applied to simulate the decays of the prefragments. The present study mainly focuses on the odd-even effect in the yields of the final fragments. We find that the odd-even effect appears in the deexcitation process of the excited prefragments, and is affected by the excitation energies and the isotope distributions of the prefragments. Both the projectile-isospin-dependent odd-even effect in the region of $-4 \leqslant T_Z \leqslant 1$ and the role of the symmetry energy on the odd-even effect are studied. We find that the odd-even effect depends sensitively on the symmetry energy.

DOI: 10.1103/PhysRevC.83.014608 PACS number(s): 25.70.Mn, 25.70.Pq, 24.10.Lx

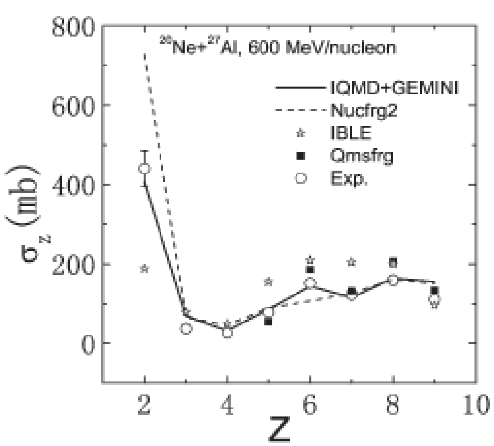


FIG. 1. Fragment cross sections presented as charge distribution for the reaction of ^{20}Ne + ^{27}Al at 600 MeV/nucleon. The experimental data [29] are shown as open circles. The calculations by the IQMD + GEMINI model are shown as a solid line. The calculations by other models are also shown: dashed line for Nucfrg2 [29], solid squares for Qmsfrg [29], and open stars for IBLE [35].

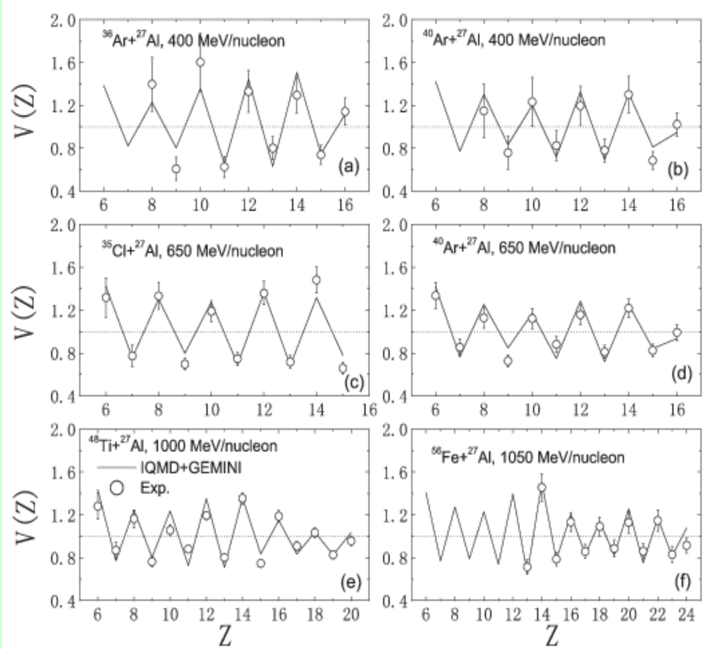


FIG. 4. Experimental $V(Z)$ (open circles) for fragments produced from the same reactions as in Fig. 2, plotted in comparison with the calculations by the IQMD + GEMINI model (solid lines).

PHYSICAL REVIEW C **84**, 037601 (2011)

Isotopic dependence of nuclear temperatures

Jun Su[1,2] and Feng-Shou Zhang[1,2,3,*]

[1] *The Key Laboratory of Beam Technology and Material Modification of Ministry of Education, College of Nuclear Science and Technology, Beijing Normal University, Beijing 100875, China*

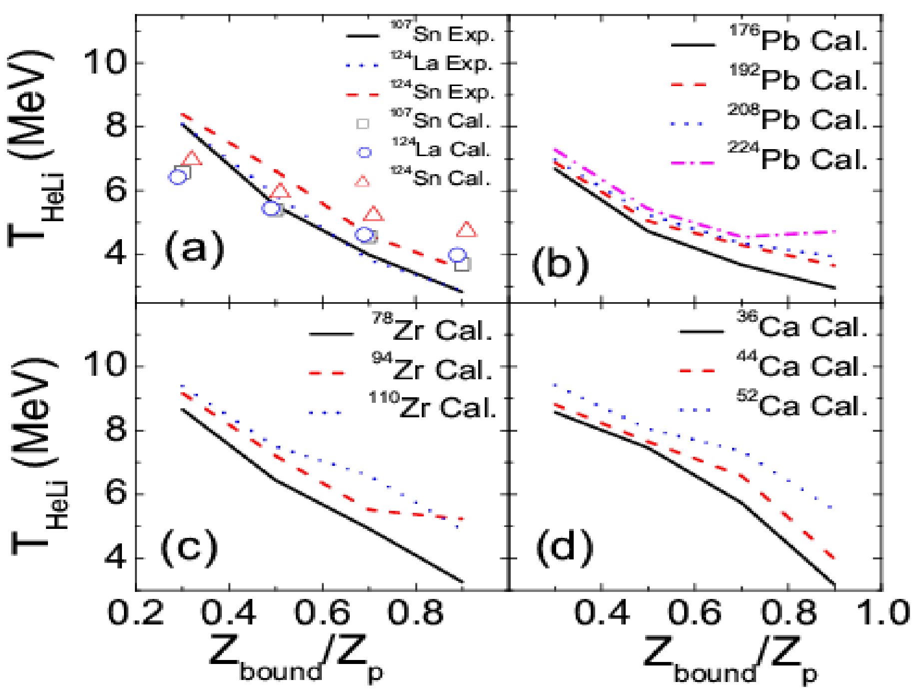
[2] *Beijing Radiation Center, Beijing 100875, China*

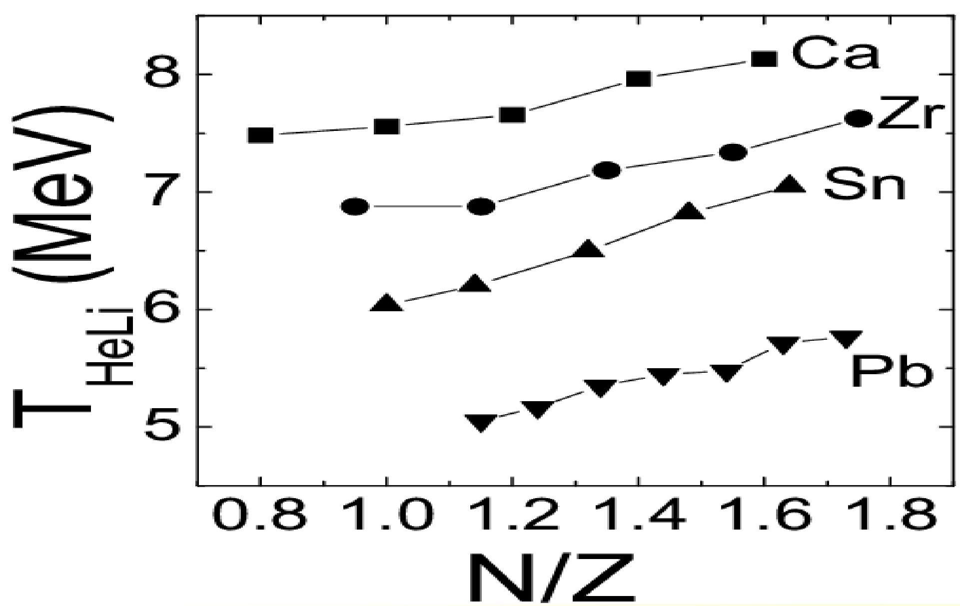
[3] *Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator of Lanzhou, Lanzhou 730000, China*

(Received 28 June 2011; published 1 September 2011)

A systematic study of isotope temperatures has been presented for heavy-ion collisions at 600 MeV/nucleon via the isospin-dependent quantum molecular dynamics model in the company of the statistical decay model (GEMINI). We find that the isospin dependence of the isotope temperatures in multifragmentation is weak; however, this effect is still visible over a wide isotopic range. The isotope temperatures for the neutron-rich projectiles are larger than those for the neutron-poor projectiles. We also find that the isotope temperatures calculated by the model decrease with increasing nuclear mass.

DOI: 10.1103/PhysRevC.84.037601 PACS number(s): 25.70.Mn, 25.70.Pq, 24.10.Lx

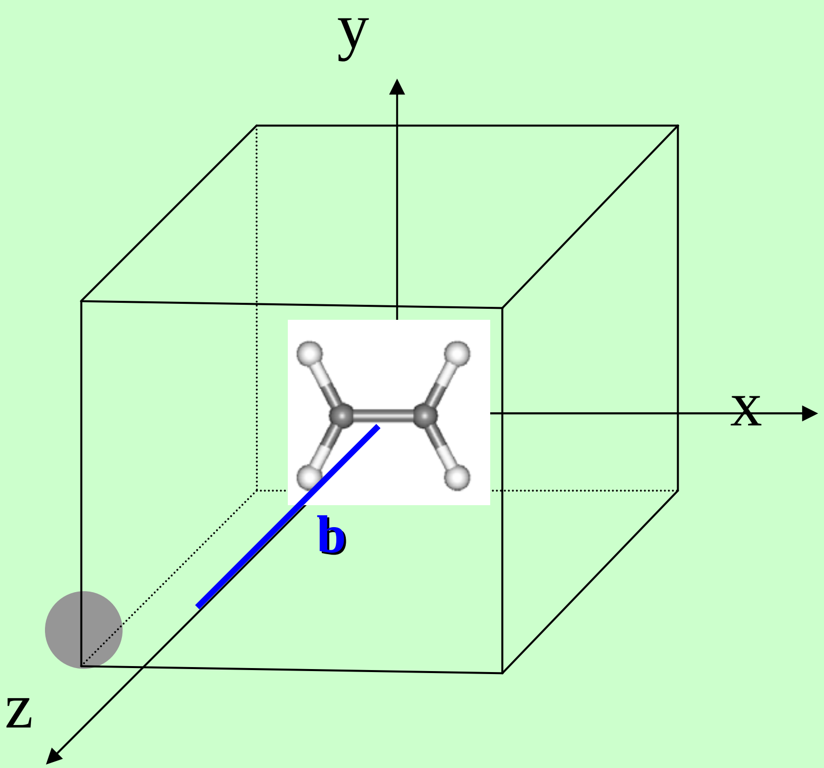




^{107}Sn, ^{124}Sn, ^{124}La (600MeV/u)+^{124}Sn

(2) Electron excitations and ionic motions

$HI + C_2H_4$ molecule



Energy (velocity)

Impact parameter

Charge

Orientation

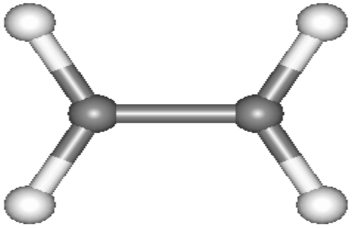
International Journal of Quantum Chemistry, Vol 111, 480–486 (2011)

Nonadiabatic Effects in the Irradiation of Ethylene

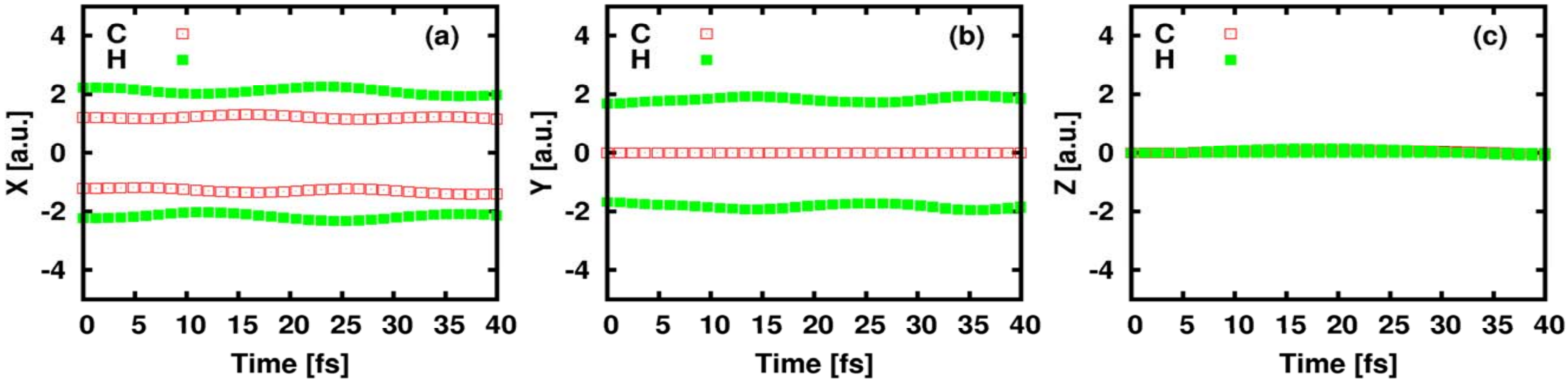
ZHI-PING WANG,[1,2,3,4,5] PHUONG MAI DINH,[4,5] PAUL GERHARD REINHARD,[6] ERIC SURAUD,[4,5] FENG SHOU ZHANG[2,3]

[1] *School of Science, JiangNan University, Wuxi 214122, China*
[2] *The Key Laboratory of Beam Technology and Material Modification of Ministry of Education, College of Nuclear Science and Technology, Beijing Normal University, Beijing 100875, People's Republic of China*
[3] *Beijing Radiation Center, Beijing 100875, China*
[4] *Université de Toulouse, UPS, Laboratoire Physique Théorique (IRSAMC), F-31062 Toulouse, France*
[5] *CNRS, LPT(IRSAMC), F-31062 Toulouse, France*
[6] *Institut für Theoretische Physik, Universität Erlangen, Staudtstrasse 7, D-91058 Erlangen, Germany*

Received 15 January 2010; accepted 9 February 2010
Published online 2 June 2010 in Wiley Online Library (wileyonlinelibrary.com).
DOI 10.1002/qua.22656



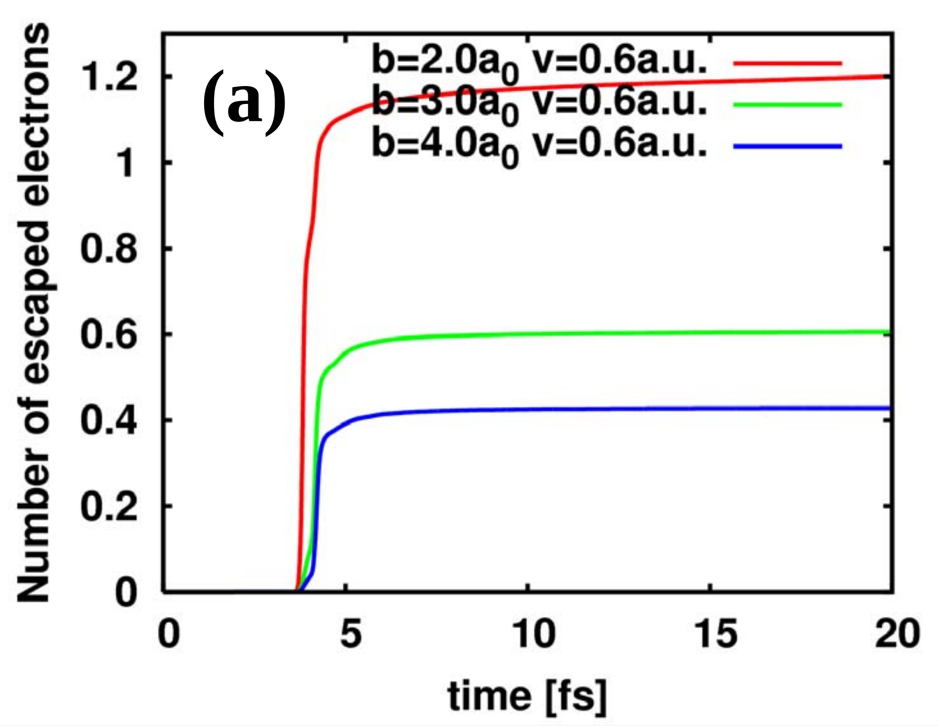
Collision process $Q = 2, b = 7a_0$

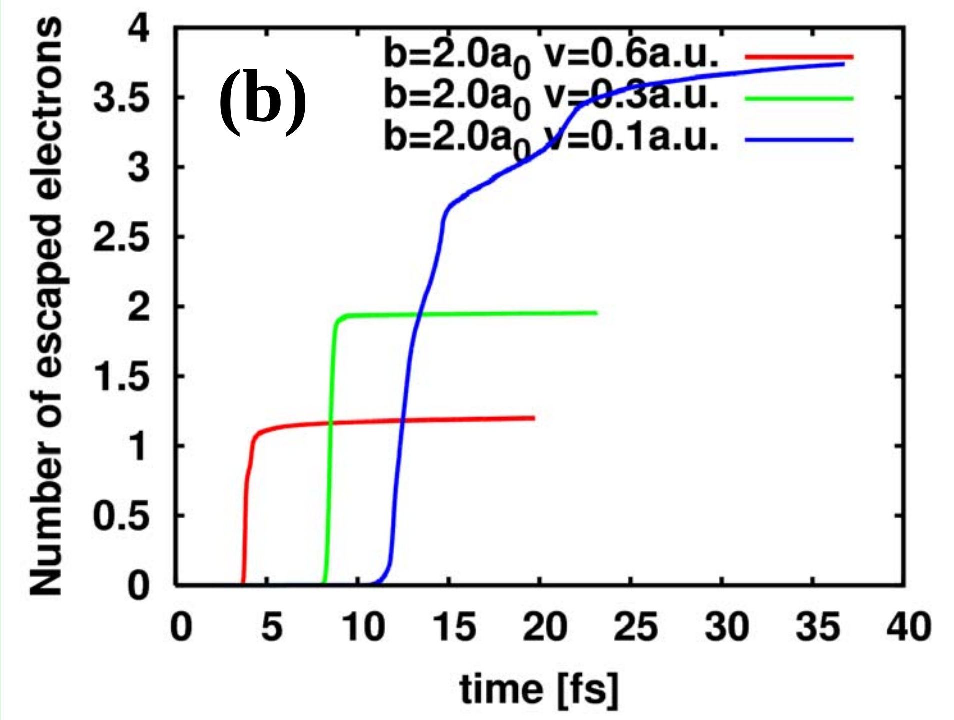


b and v dependence

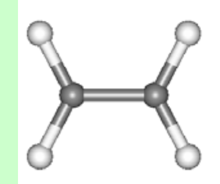
(a)influence of impact parameter b

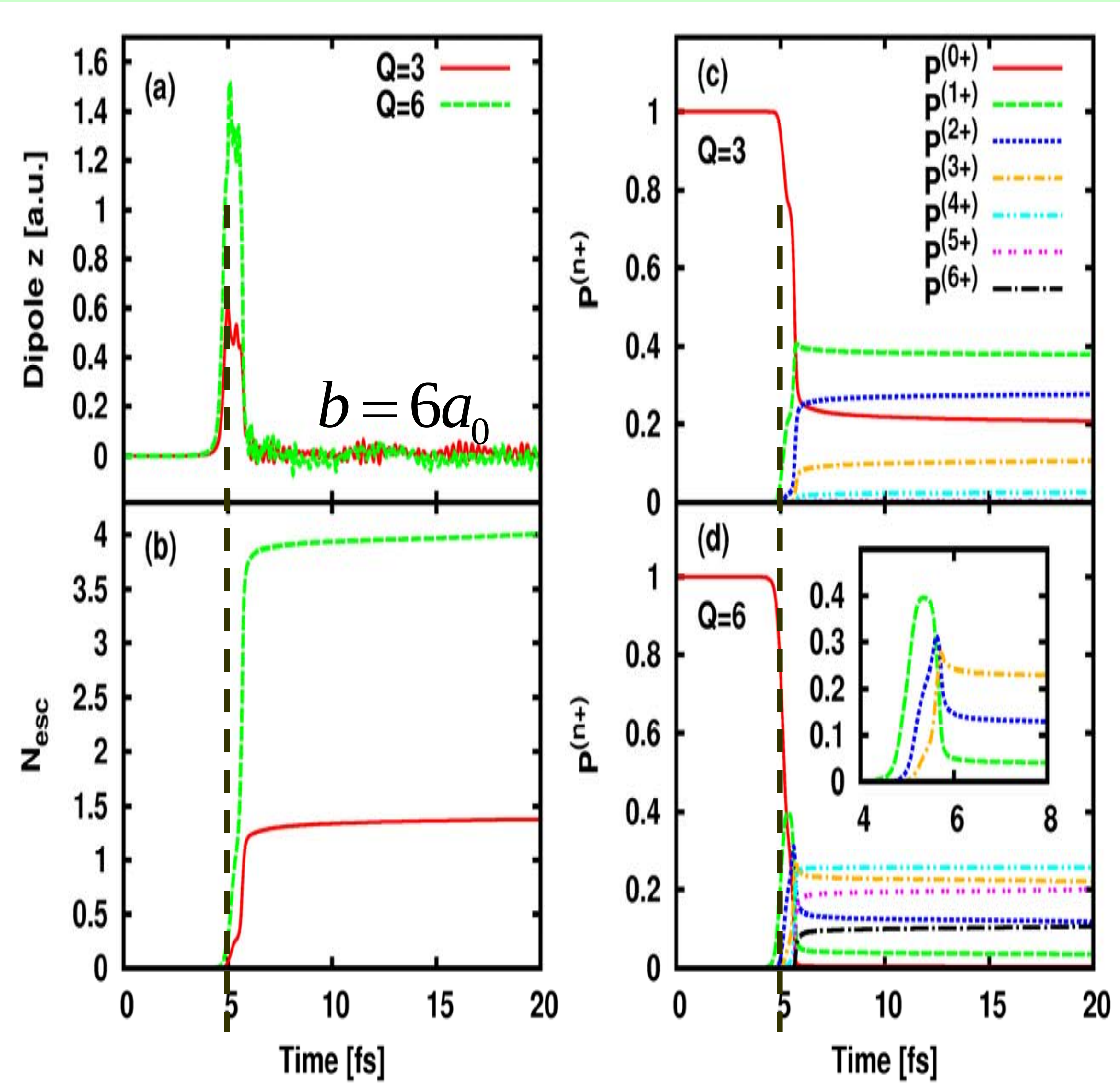
(b)influence of velocity υ

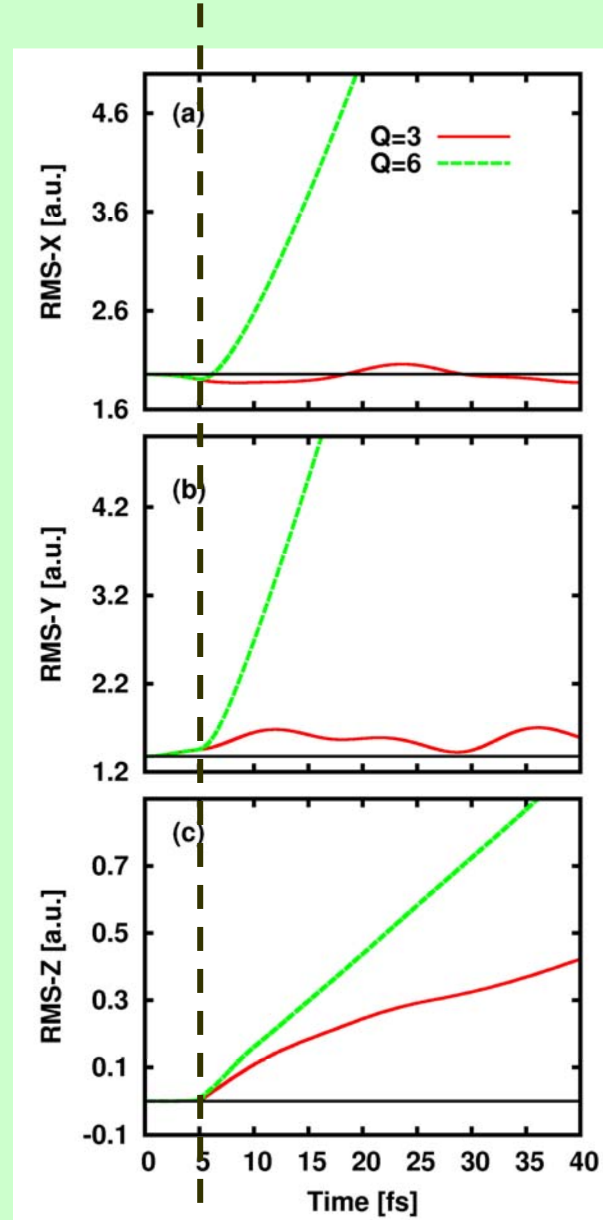




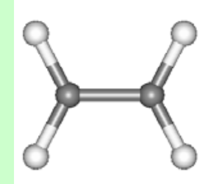
Different charges $Q=3$ $Q=6$



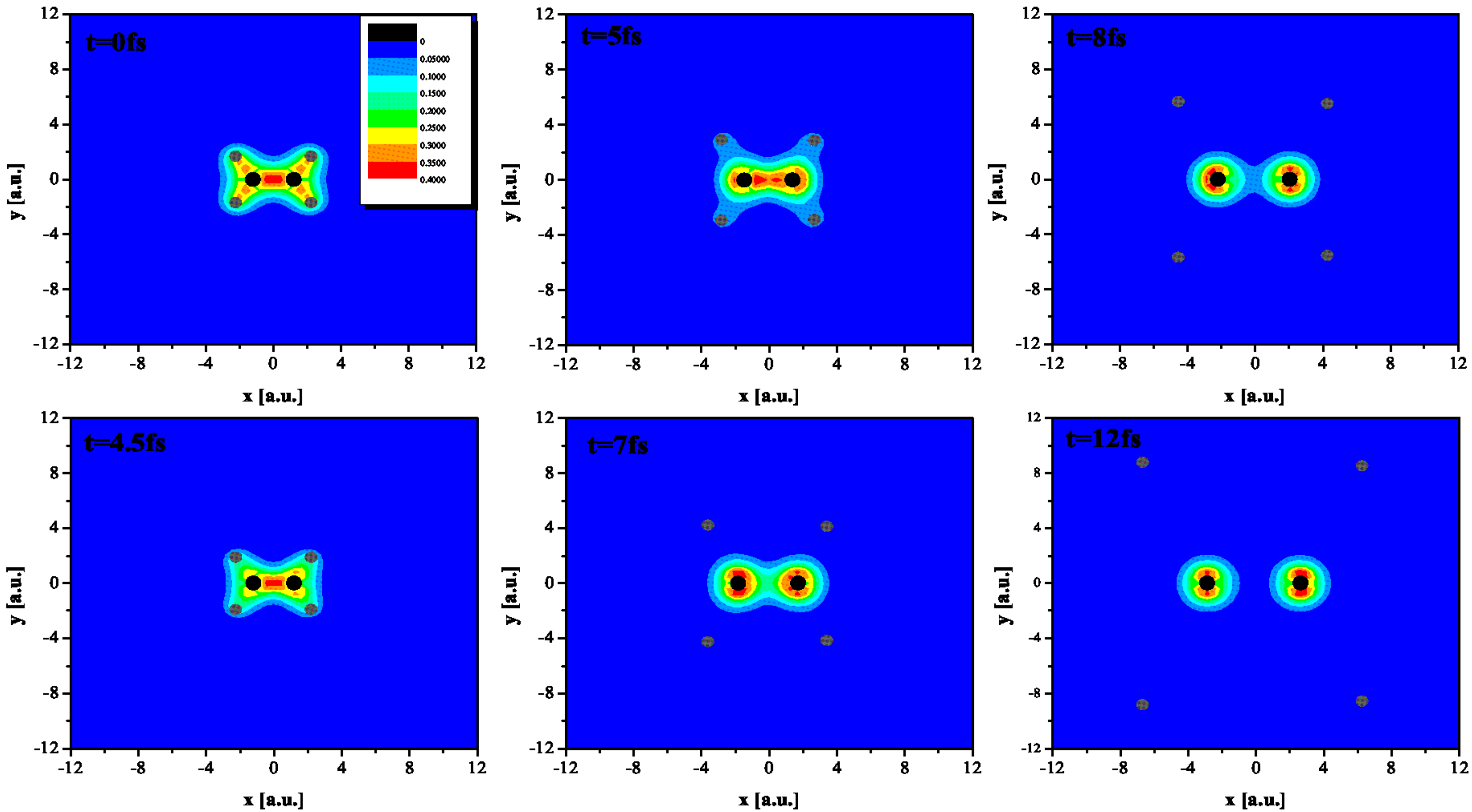




C_2H_4 Explosion at Q=6

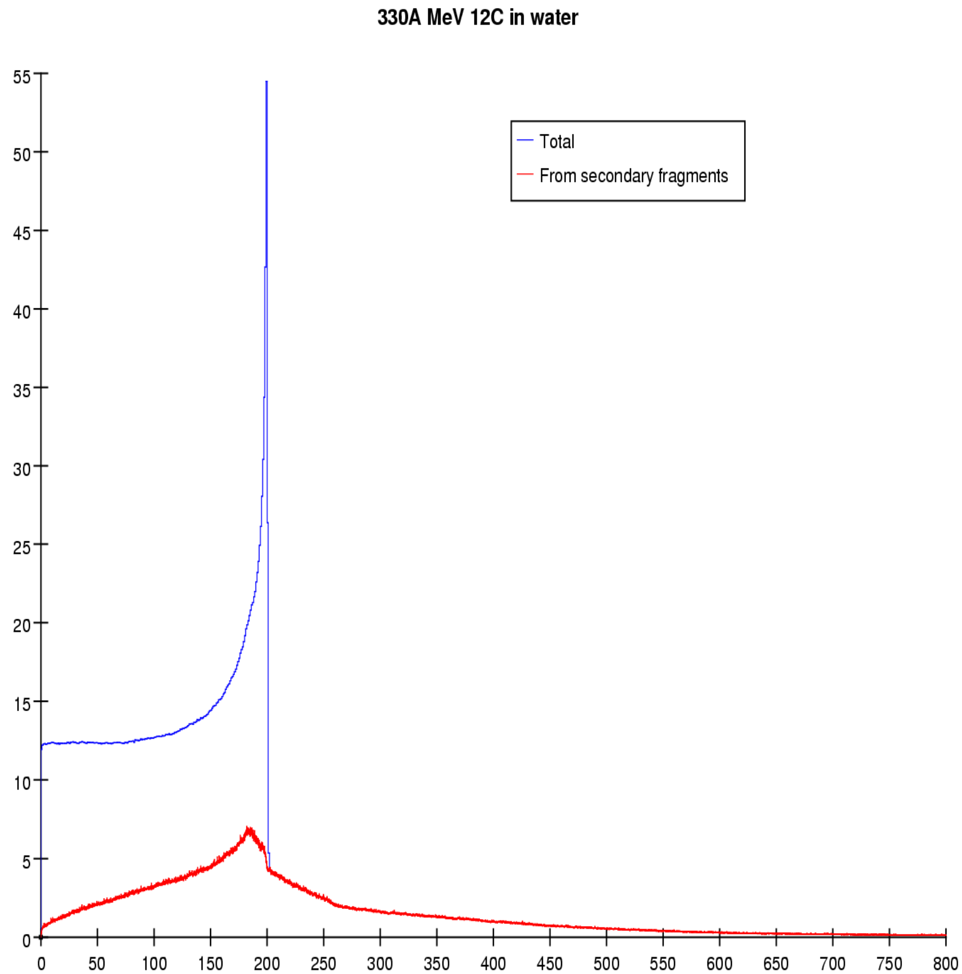


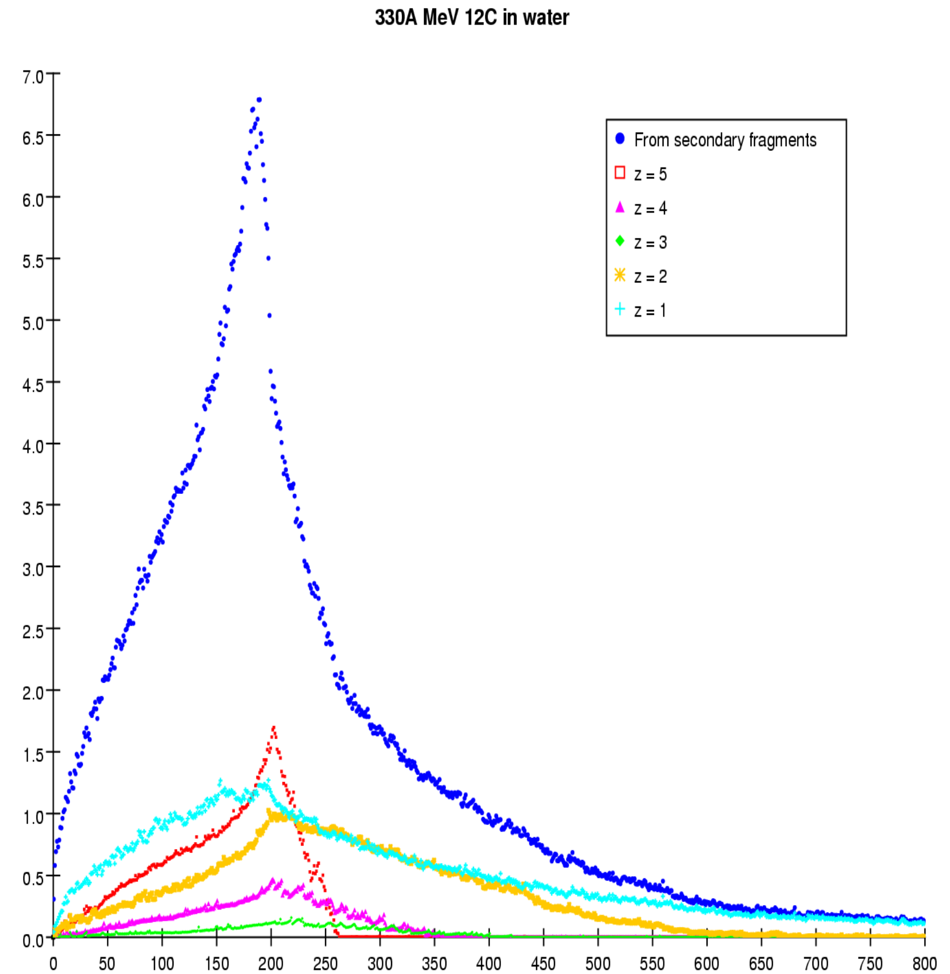
y



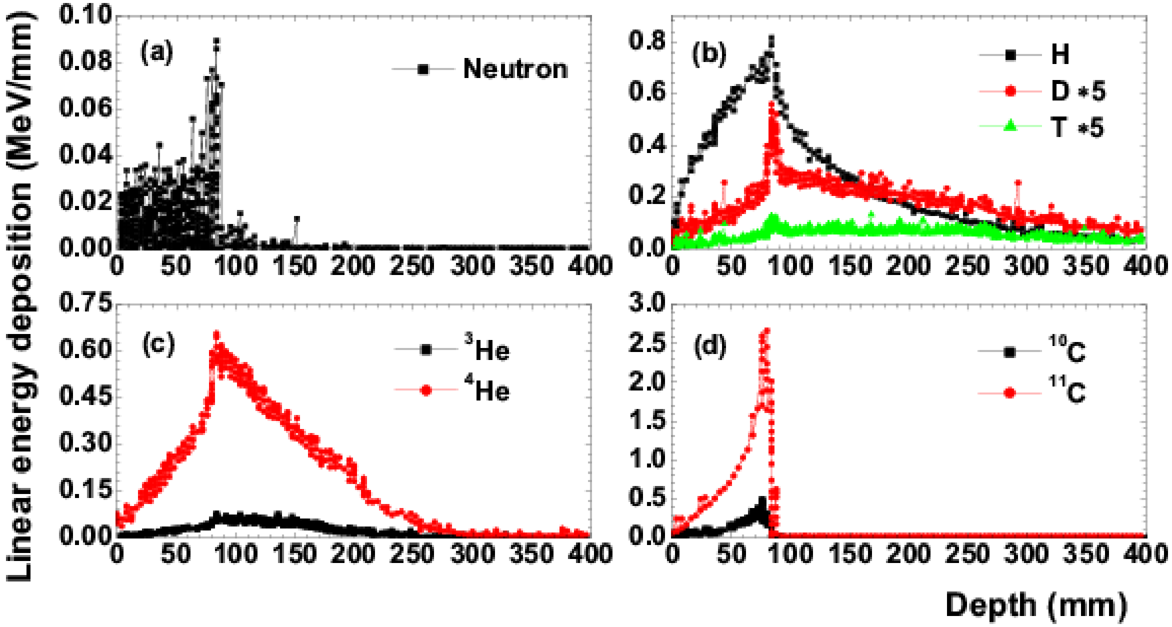
(3). Dose distributions

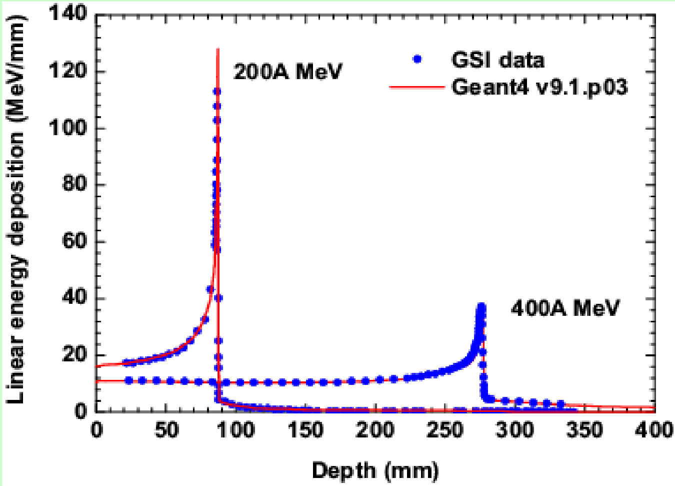
Contribution to the total energy deposition from secondary fragments produced in nuclear interactions of 330 MeV/u Carbon in water (Linear Energy Deposition as a function of penetration depth)

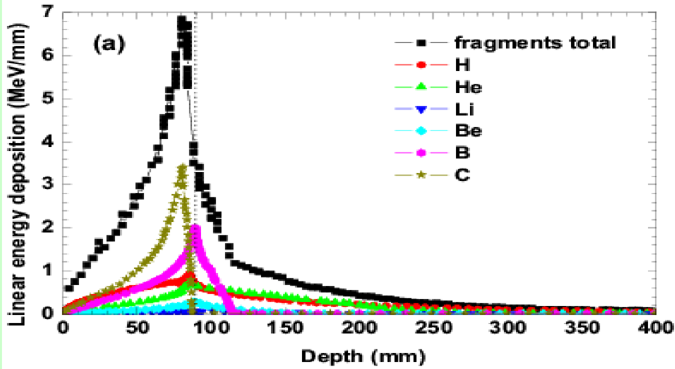


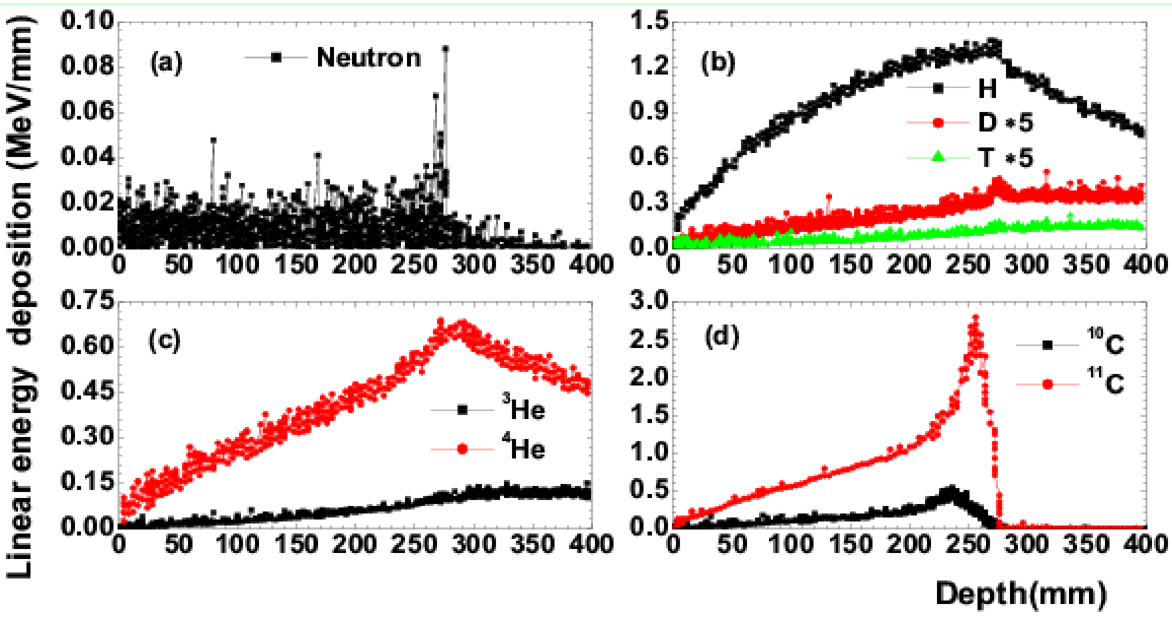


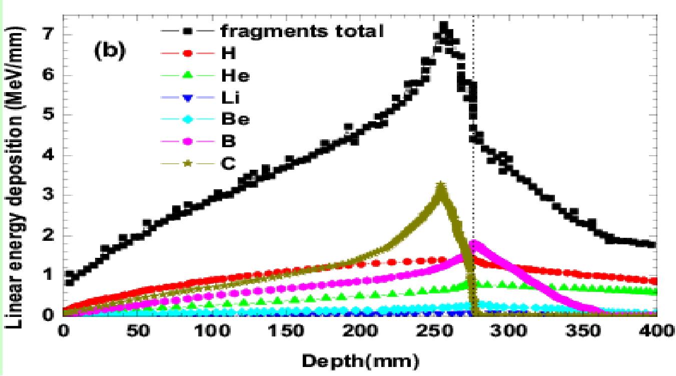
Secondary beam fragments produced by 200 and 400 MeV/u C^{6+} ions in water

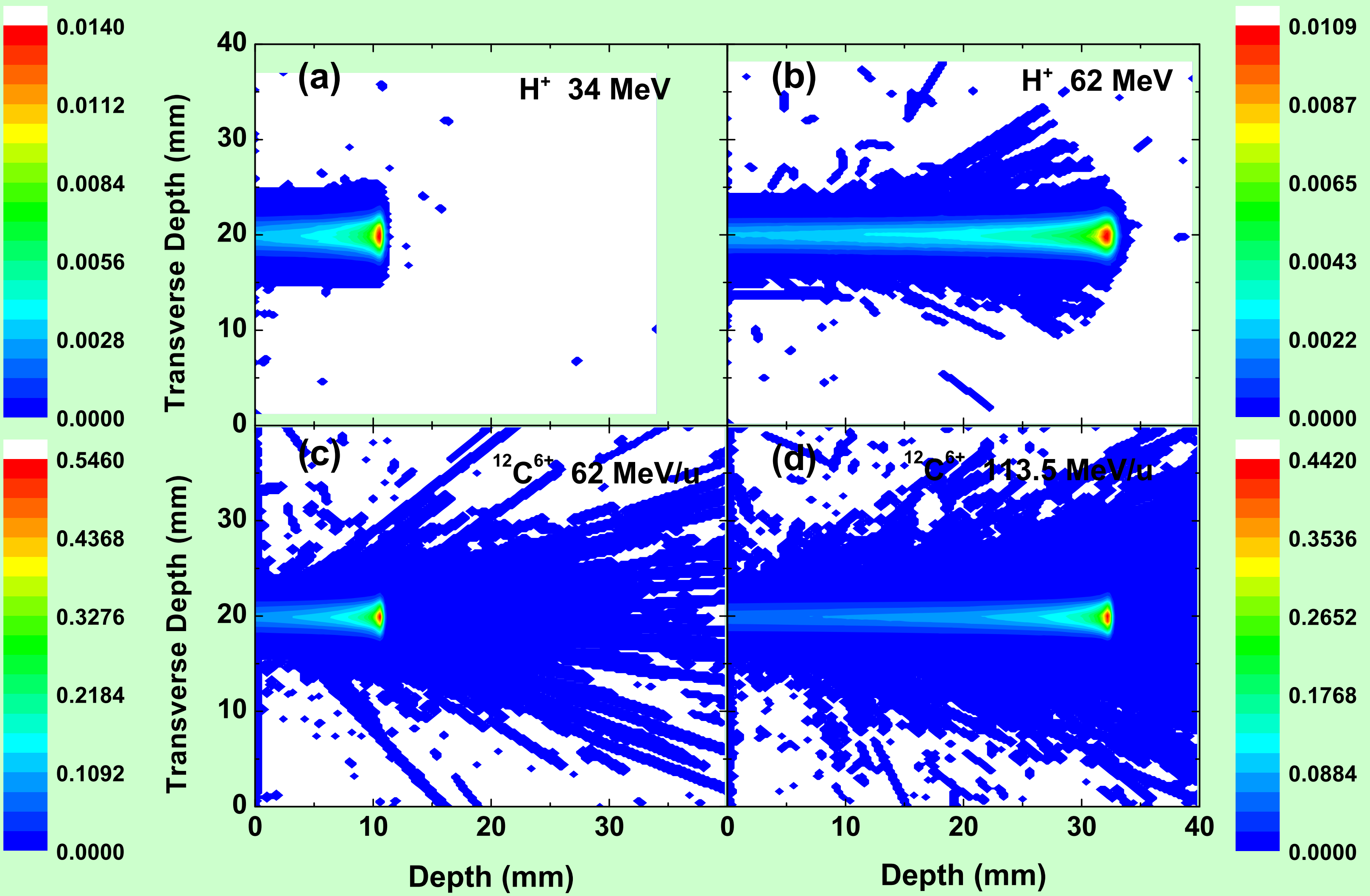










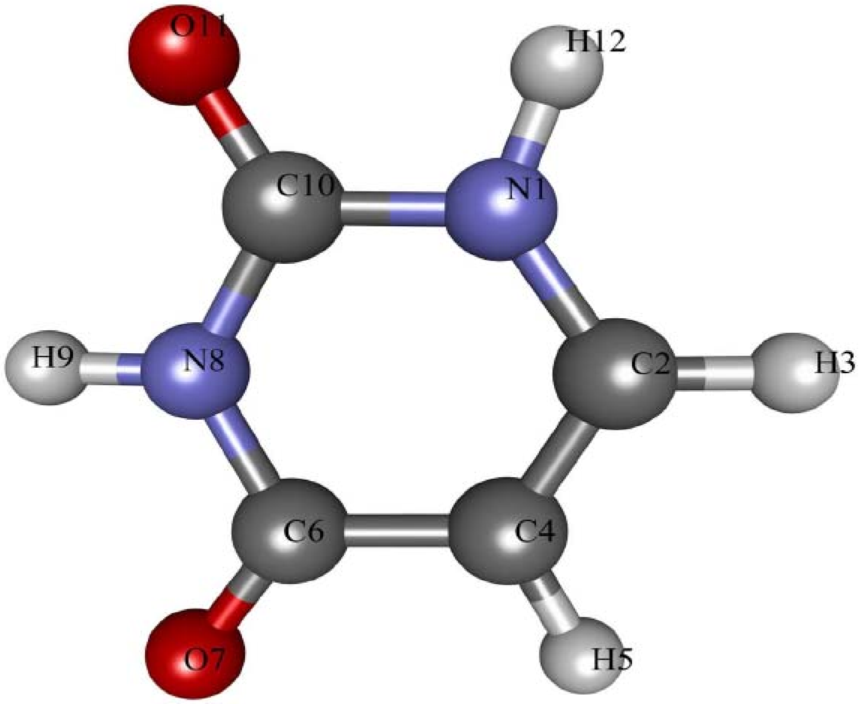

0.0140
0.0112
0.0084
0.0056
0.0028
0.0000
0.5460
0.4368
0.3276
0.2184
0.1092
0.0000
Transverse Depth (mm)
Transverse Depth (mm)
(a)
H+ 34 MeV
(b)
H+ 62 MeV
(c)
12C6+ 62 MeV/u
(d)
12C6+ 113.5 MeV/u
Depth (mm)
Depth (mm)
0.0109
0.0087
0.0065
0.0043
0.0022
0.0000
0.4420
0.3536
0.2652
0.1768
0.0884
0.0000

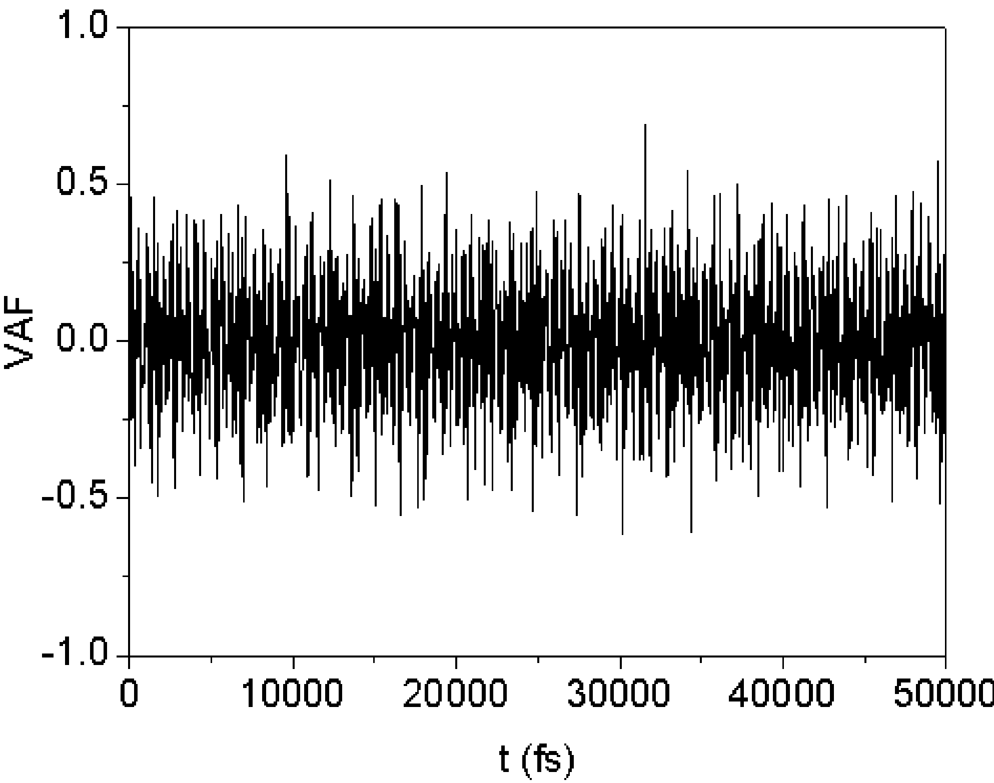
（4）Structure properties of biomolecule: U

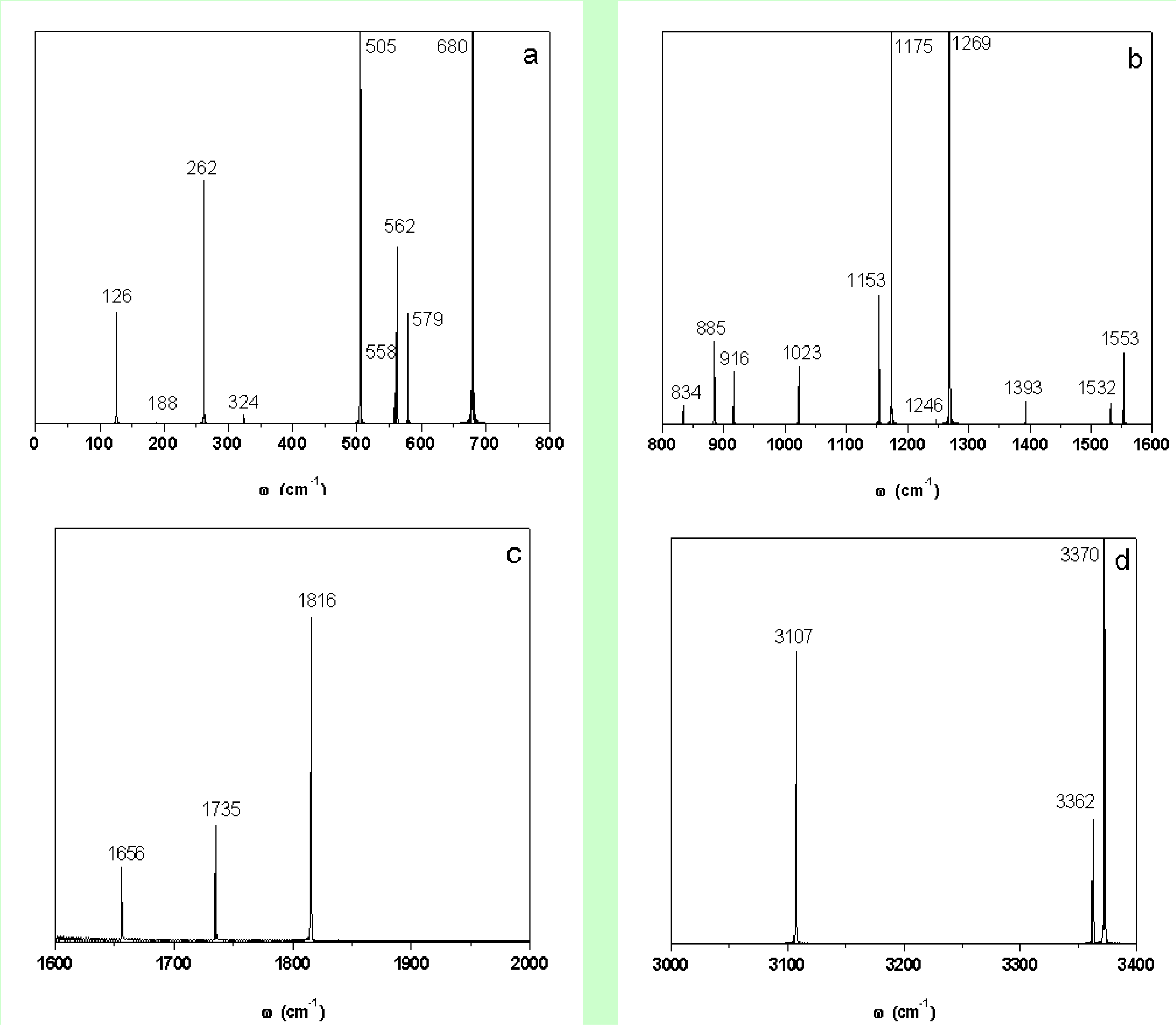
（Wang, Zhang, Gu, Zhou，

Chinese Science Bulletin 51(2006)1804)

Structure of Uracil





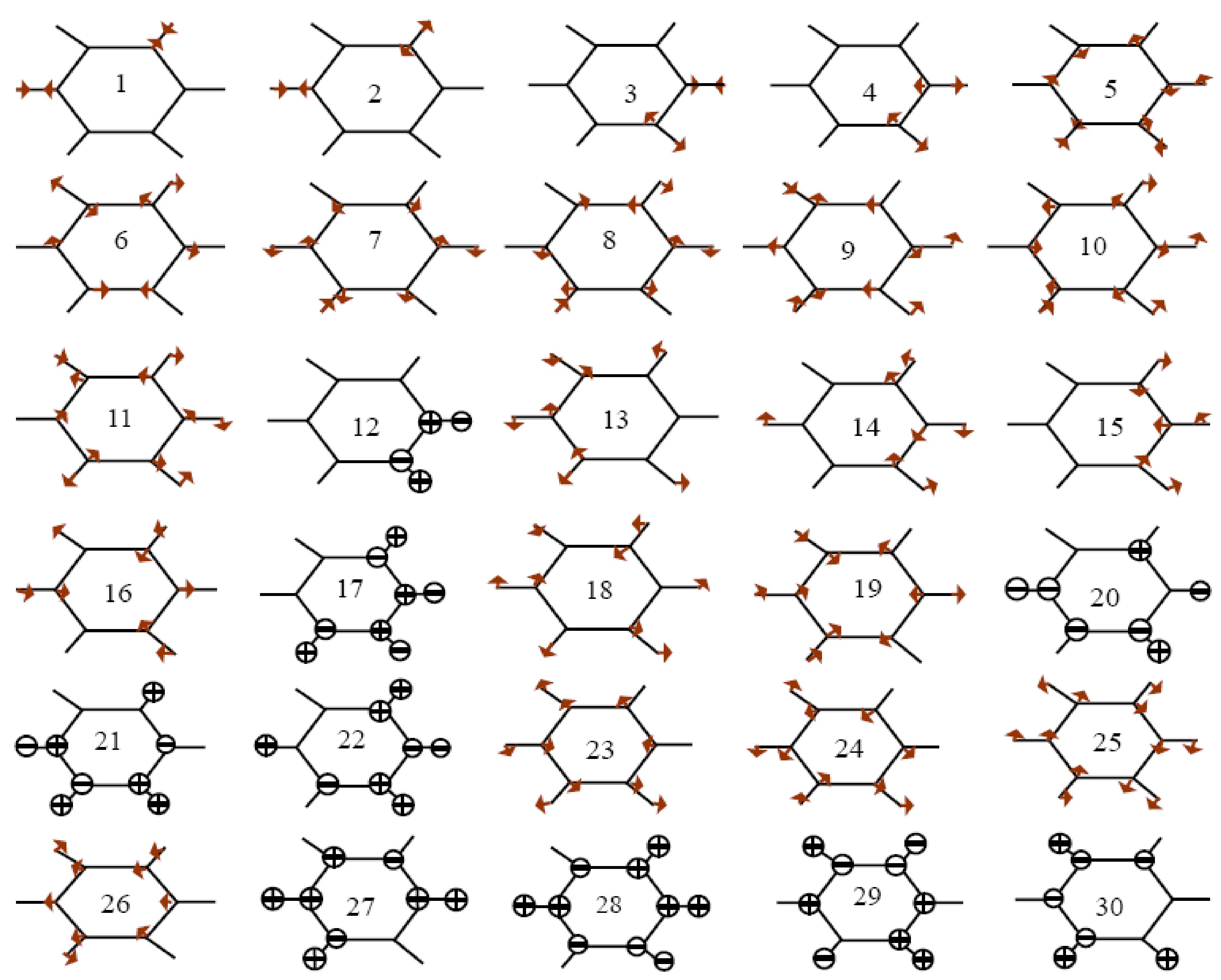

a
505
680
262
562
126
579
558
188
324
0
100
200
300
400
500
600
700
800
ω (cm⁻¹)
b
1175
1269
1153
885
916
1023
1553
834
1393
1532
1246
800
900
1000
1100
1200
1300
1400
1500
1600
ω (cm⁻¹)
c
1816
1735
1656
1600
1700
1800
1900
2000
ω (cm⁻¹)
d
3370
3107
3362
3000
3100
3200
3300
3400
ω (cm⁻¹)

Vibrational frequencies of Uracil

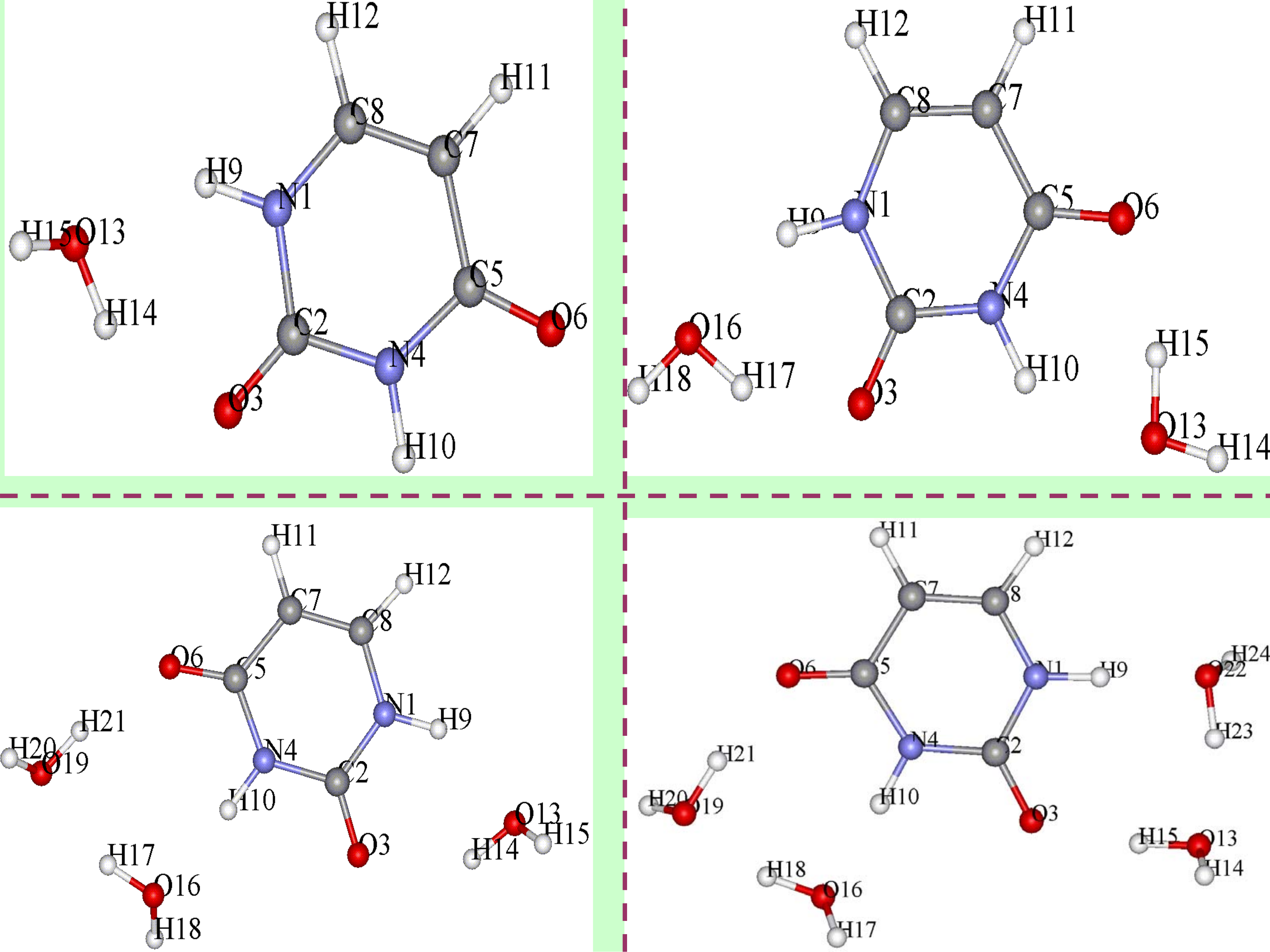
Mode	FDH	VAF	Infrared		Raman*	B3LYP/6-31G (d,p)*	Mode	FDH	VAF	Infrared		Raman*	B3LYP/6-31G (d,p)*
			Ar Matrix*	gas*						Ar Matrix*	gas*		
1	3330	3370	3485	3484		3658	16	916	916	980	972	994	970
2	3321	3362	3435	3436		3620	17	888	885	958	952	928	965
3	3085			3124		3264	18	835	834	804	802	860	813
4	3077	3107		3076		3221	19	713		759		824	772
5	1809	1816	1764	1756	1706	1845	20	683	680	757	757	804	752
6	1729	1735	1706	1703	1679	1808	21	582	579	718	717	786	729
7	1652	1656	1643	1641	1645	1690	22	564	562	662	660	761	687
8	1550	1553	1472	1461	1520	1506	23	559	558	562	545	579	563
9	1528	1532	1400	1400	1502	1422	24	530	529	551		563	558
10	1393	1393	1389	1387	1456	1407	25	506	505	537			541
11	1270	1269	1359	1356	1392	1382	26	357	356	516	512	530	519
12	1249	1246	1217	1228	1260	1231	27	325	324	411	395		396
13	1176	1175	1185	1172	1233	1198	28	263	262	391	374	429	385
14	1157	1153	1075	1082	1100	1091	29	189	188	185	185	195	170
15	1025	1023	987	990	1006	990	30	127	126	119		145	150

Experimental data:

1. Graindourze, Grootaers, Smets, et al. J. Mol. Str.(Theochem), 237(1990)389
2. Palafox, Rastogi, Spectrochim Acta， A58 (2002)411
3. Florian, Hrouda, Spectrochim Acta, A49(1993)921



eigen modes of Uracil


H12
H11
C8
C7
H9
N1
H15
O13
C5
H14
C2
O6
N4
O3
H10
H12
H11
C8
C7
N1
C5
O6
C2
N4
O16
H15
H18
H17
H10
O13
H14
H11
H12
C7
O6
N1
H9
H21
H20
O19
N4
C2
H10
O13
H15
O3
H14
H17
O16
H18
H11
H12
H24
H9
H21
N4
H23
H10
O3
H15
O13
H18
O16
H14
H17

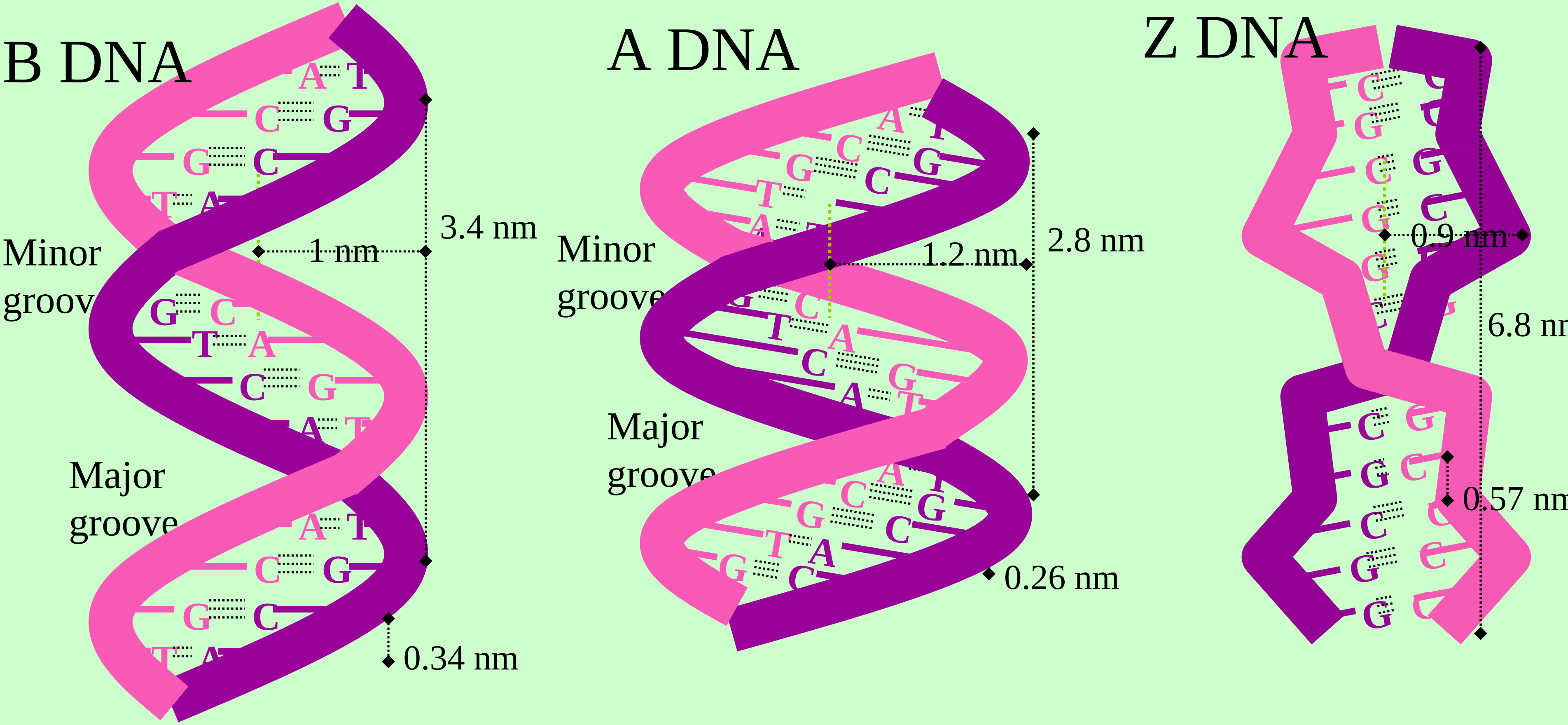
Vibrational frequencies of hydrated Uracil (in cm^{-1}) (only vibration of U molecule)

Mode	uracil	Uw's U	U2w's U	U3w's U	U4w's U
1	3330	3323	3322	3313	3299
2	3321	3313	3290	3286	3206
3	3085	3076	3061	3063	3008
4	3077	3068	3052	3053	2965
5	1809	1807	1814	1815	1860
6	1729	1729	1740	1740	1759
7	1652	1650	1656	1655	1656
8	1550	1548	1556	1552	1578
9	1528	1527	1533	1534	1515
10	1393	1388	1413	1414	1424
11	1270	1270	1316	1312	1392
12	1249	1230	1251	1251	1356
13	1176	1158	1213	1214	1309
14	1157	1137	1185	1184	1285
15	1025	1021	1054	1055	1262

Mode	uracil	Uw's U	U2w's U	U3w's U	U4w's U
16	916	910	1005	1004	1219
17	888	873	937	938	1174
18	835	815	930	937	1139
19	713	741	881	912	1053
20	683	707	852	864	951
21	582	563	732	734	869
22	564	553	593	594	772
23	559	523	588	586	704
24	530	522	560	565	691
25	506	494	508	512	614
26	357	351	433	433	574
27	325	310	396	395	470
28	263	245	358	360	379
29	189	165	132	130	277
30	127	125	97	101	157

(5). Structure changes of DNA

J.Chem.Phys.135（2011）034509, X. Shen et al



10.4 Bp/turn	11 Bp/turn	12 Bp/turn
+34.6° Rotation/Bp	+34.7° Rotation/Bp	-30.0° Rotation/Bp

Even More Forms Of DNA

- **C-DNA:**
  - Exists only under high dehydration conditions
  - 9.3 bp/turn, 0.19 nm diameter and tilted bases
- **D-DNA:**
  - Occurs in helices lacking guanine
  - 8 bp/turn
- **E-DNA:**
  - Like D-DNA lack guanine
  - 7.5 bp/turn
- **P-DNA:**
  - Artificially stretched DNA with phosphate groups found inside the long thin molecule and bases closer to the outside surface of the helix
  - 2.62 bp/turn

B-DNA appears to be the most common form *in vivo*. However, under some circumstances, alternative forms of DNA may play a biologically significant role.

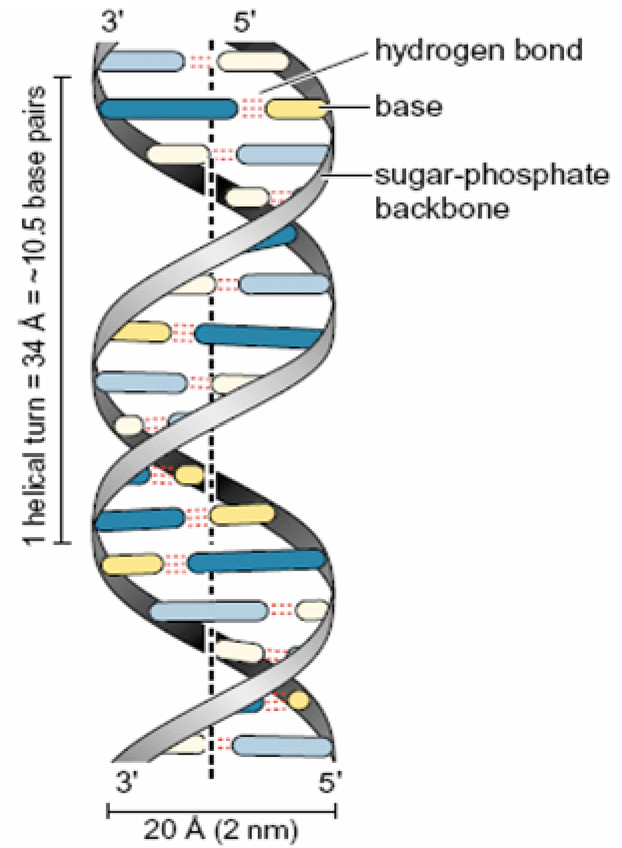
DNA conformation transition ?

Factors to keep helix of DNA

- base stacking
- hydrogen-bonds
- solvent
- counterions

Water ⇨ Solvent environment

Temperature, pressure, free radical, etc.



What we most care for?

"Knowing **which properties of water are particularly sensitive to its structure** can help to show how fine-tuned for life the liquid properties are"

NATURE Vol .436 25 August 2005

"water in changing", "counterions in changing", "temperature in changing"

PRL 100, 088104 (2008) PHYSICAL REVIEW LETTERS week ending 29 FEBRUARY 2008

Solvent-Induced DNA Conformational Transition

B. Gu,[1,2] F. S. Zhang,[1,2,3,*] Z. P. Wang,[1,2] and H. Y. Zhou[1,2]

[1]*The Key Laboratory of Beam Technology and Material Modification of Ministry of Education, Institute of Low Energy Nuclear Physics, Beijing Normal University, Beijing 100875, China*

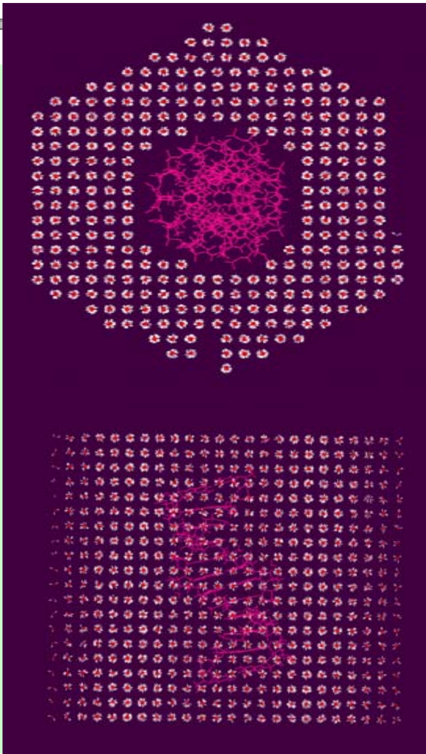
[2]*Beijing Radiation Center, Beijing 100875, China*

[3]*Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator of Lanzhou, Lanzhou 730000, China*

(Received 15 October 2007; published 29 February 2008)

Modified water models with scaled charges are used to investigate solvent polarity effects on DNA structure. Several intensive molecular dynamics simulations of the DNA EcoRI dodecamer d(CGCGAATTCGCG) in different model solvents are performed. When the polarity of the solvent molecule decreases, from overpolarized to less polarized, DNA experiences the conformational transitions of constrained → *B* form → (*A*-*B*)mix → *A* form. We demonstrate that one important cause of these structure changes is the competition between hydration and direct cation coupling to the free oxygen atoms in the phosphate groups on DNA backbones.

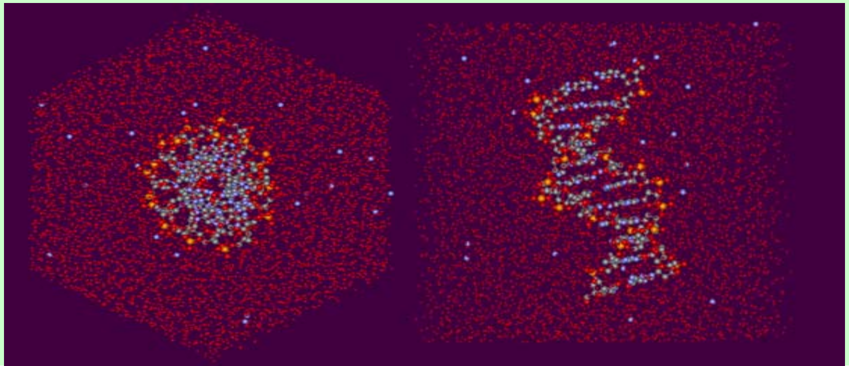
DOI: 10.1103/PhysRevLett.100.088104 PACS numbers: 87.14.G−, 61.25.Er



1 171d DNA

22 ***Na*+ neutralizing ions**

5800 **charge-scaled water**



Na^+ interacts with DNA

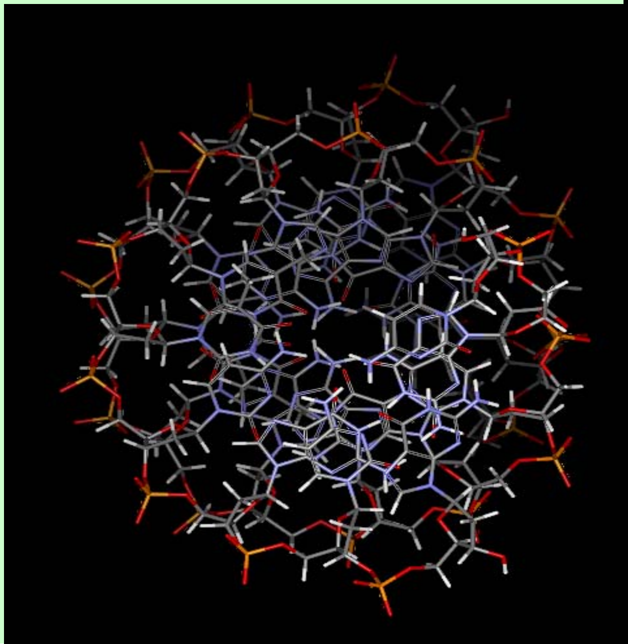
DNA： 171d PDB (Protein Date Bank)

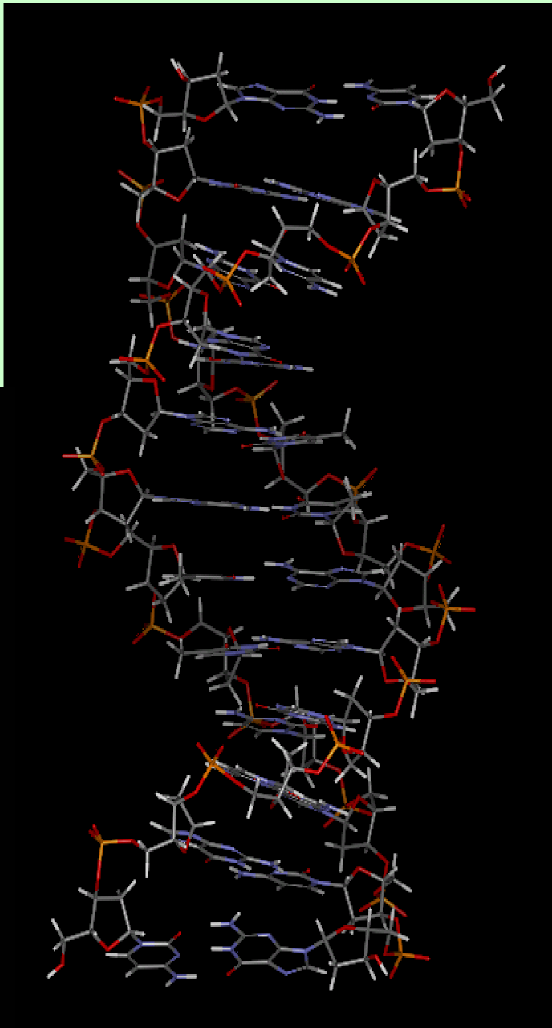
NMR structure of a synthetic B-type dodecamer

d(CGCGAATTCGCG)

One cell: Hexagonal（~60 X 60 X 58 A^3), NVT, 298 K

171d DNA (1) + Na^+ (22)neutralizing ions + H_2O（~5000）





Charge Scale

Scale	Charges(|e|) O/H	Polarity(C·m×10^{-29})
0.6	**-0.492/0.246**	**0.4551**
0.7	**-0.574/0.287**	**0.5310**
0.8	**-0.654/0.328**	**0.6068**
1.0(SPC)	**-0.820/0.410**	**0.7585**
1.2	**-0.984/0.492**	**0.9102**

Ions

Ion	**σ (A)**	**ε (kJ/mol)**
Li+	**2.37**	**0.149**
Na+	**2.73**	**0.358**
K+	**3.36**	**0.568**
Ru+	**3.36**	**0.568**
Cs+	**3.57**	**1.602**

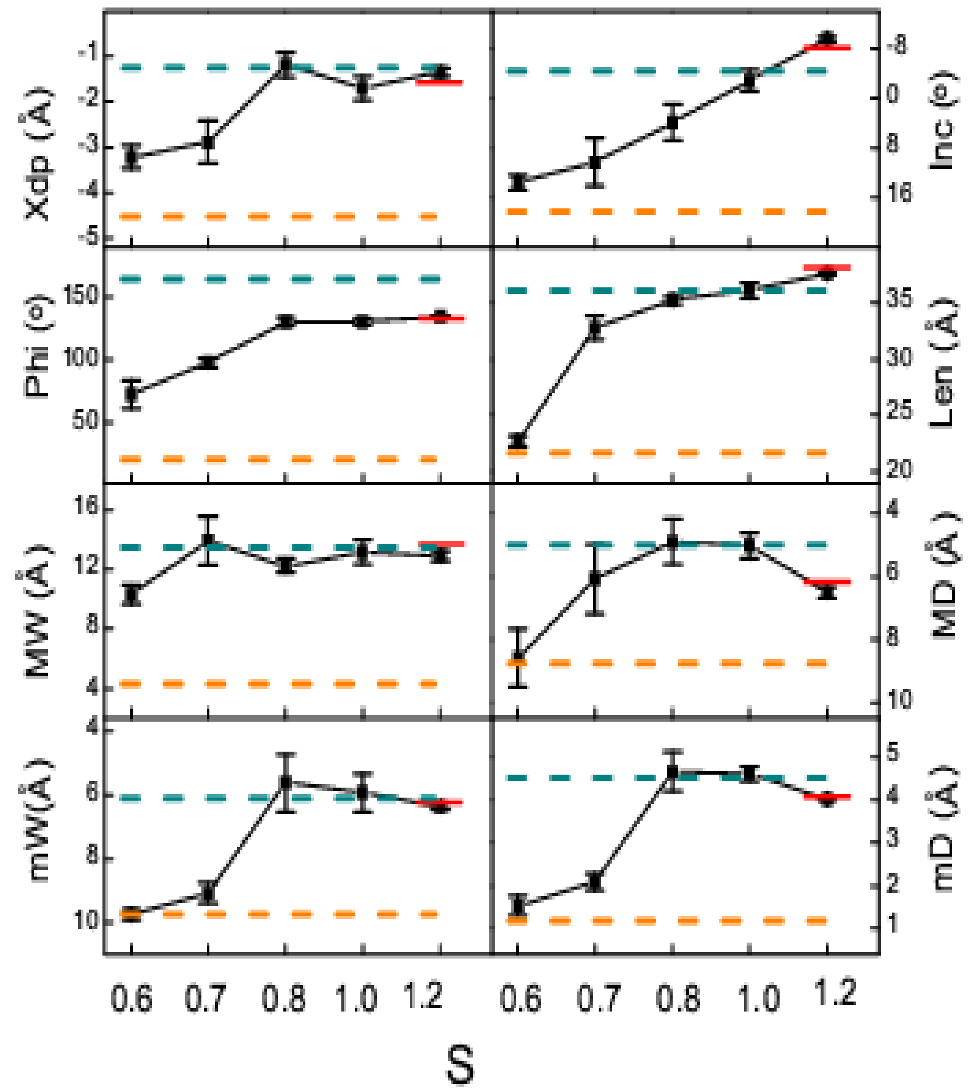
Temperature Scale

T (K)	200	260	280	298	310	343		…

Averaged DNA structure parameters (2 ns)
typical A(orange), B(blue), and starting PDB(red)

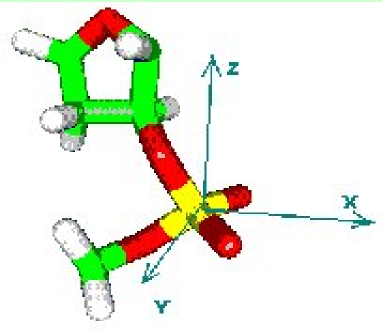
A,
B,
171d

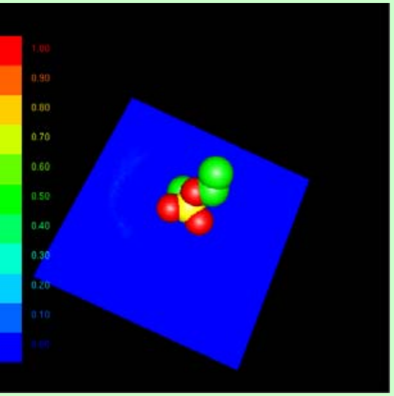
(1) x-displacement (Xdp)
(2) inclination angle (Inc) of a base-pair from helical axis,
(3) sugar pucker angle (Phi)
(4) end to end length (Len)
(5) width of Major groove MW
(6) depth of Major groove MD
(7) width of minor groove mW
(8) depth of minor groove mD



O(P)周围的Na^+

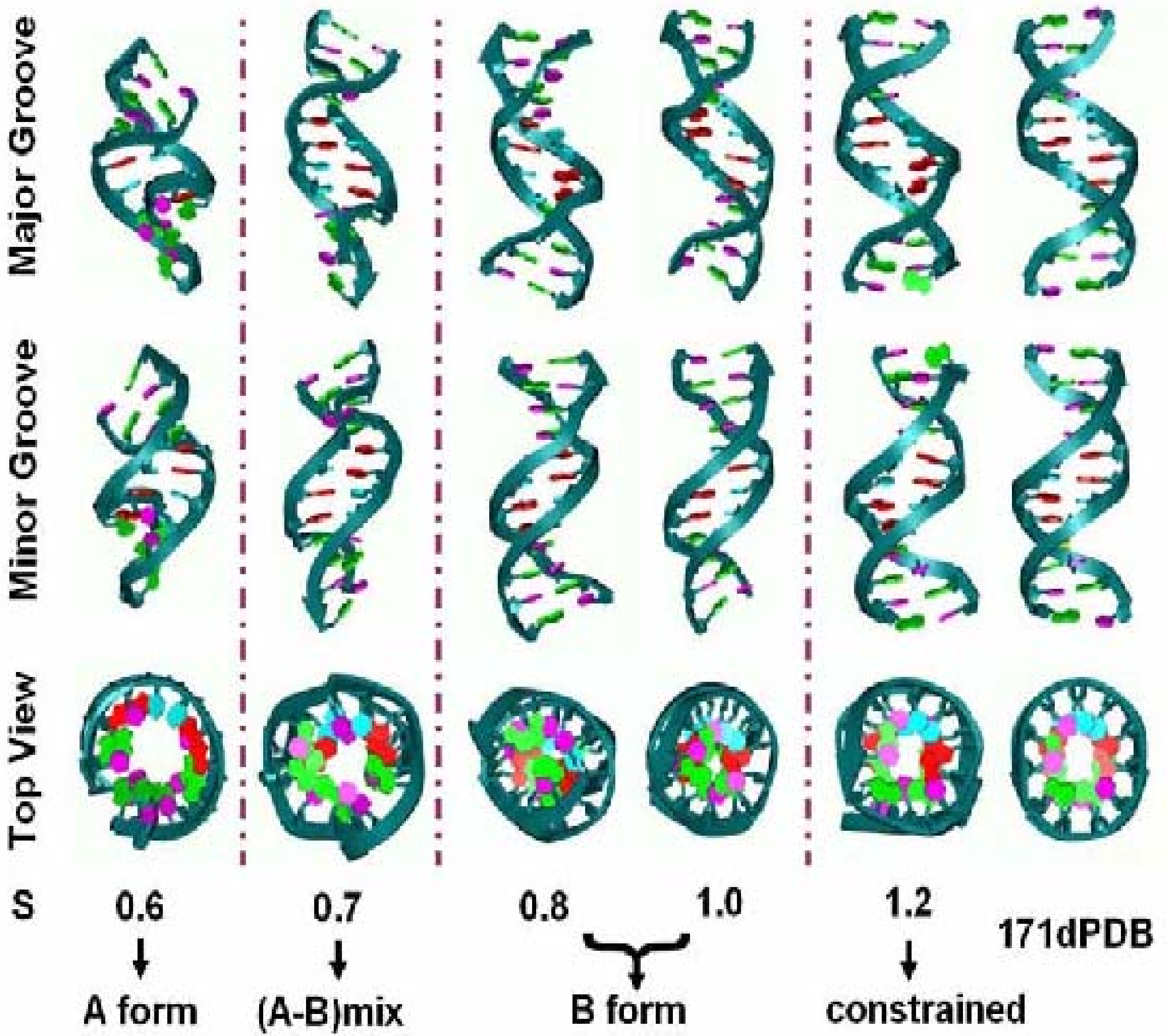
B. Gu et al., PRL100 (2008) 088104



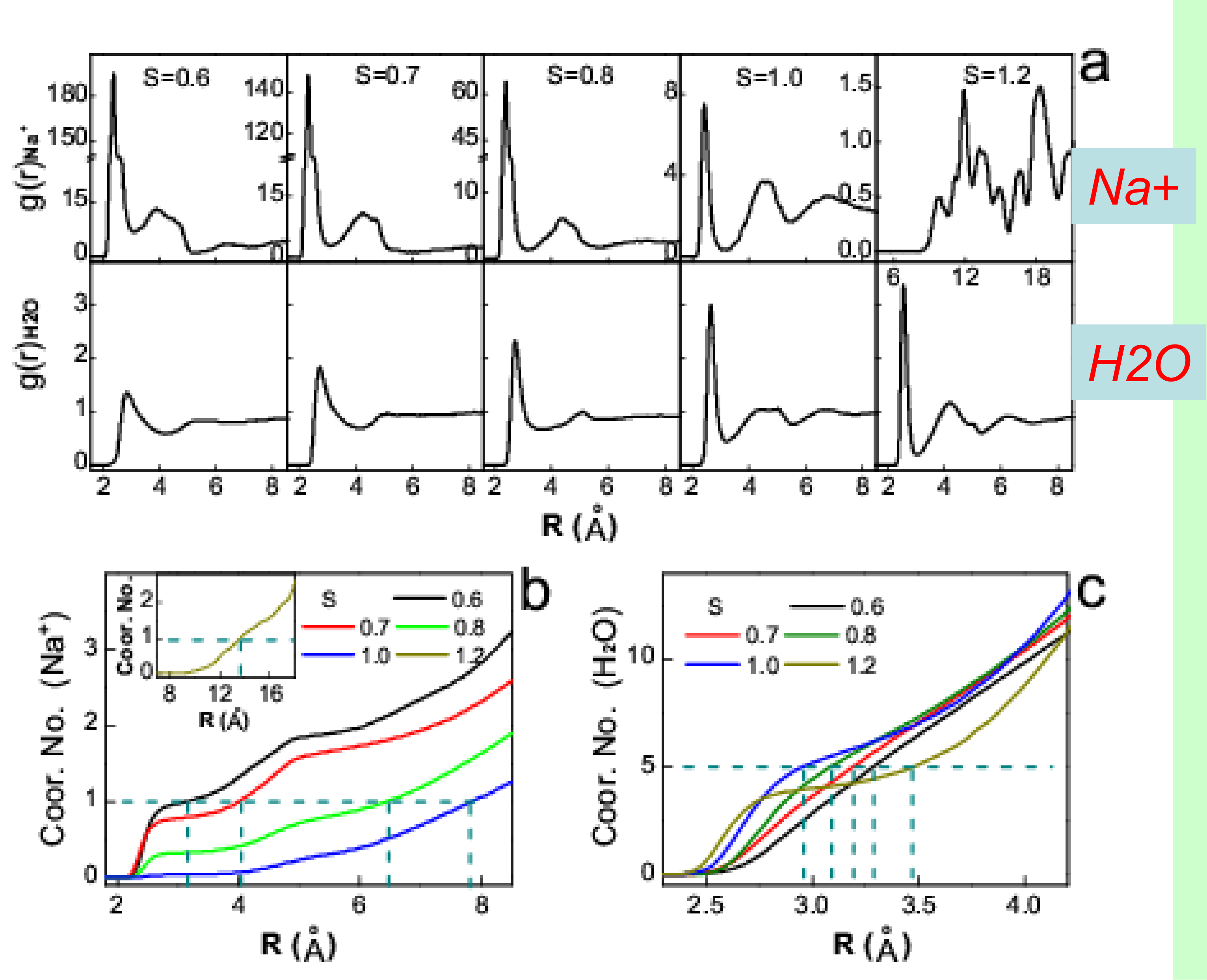


空间分布函数
x-y截面

Na^+-O(P)



Radial distribution functions (RDF) and the coordination no. of Na^+ ions and H_2O



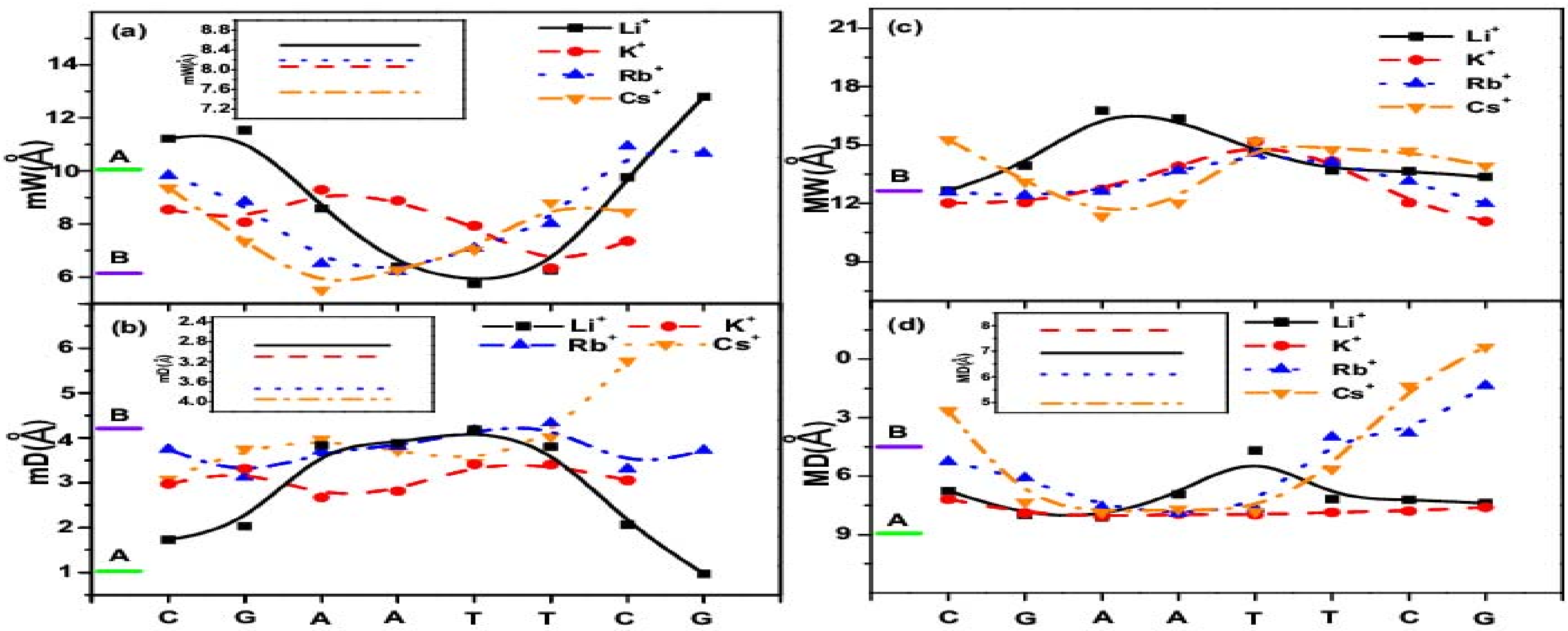
THE JOURNAL OF CHEMICAL PHYSICS **135**, 034509 (2011)

Solvent effects on the conformation of DNA dodecamer segment: A simulation study

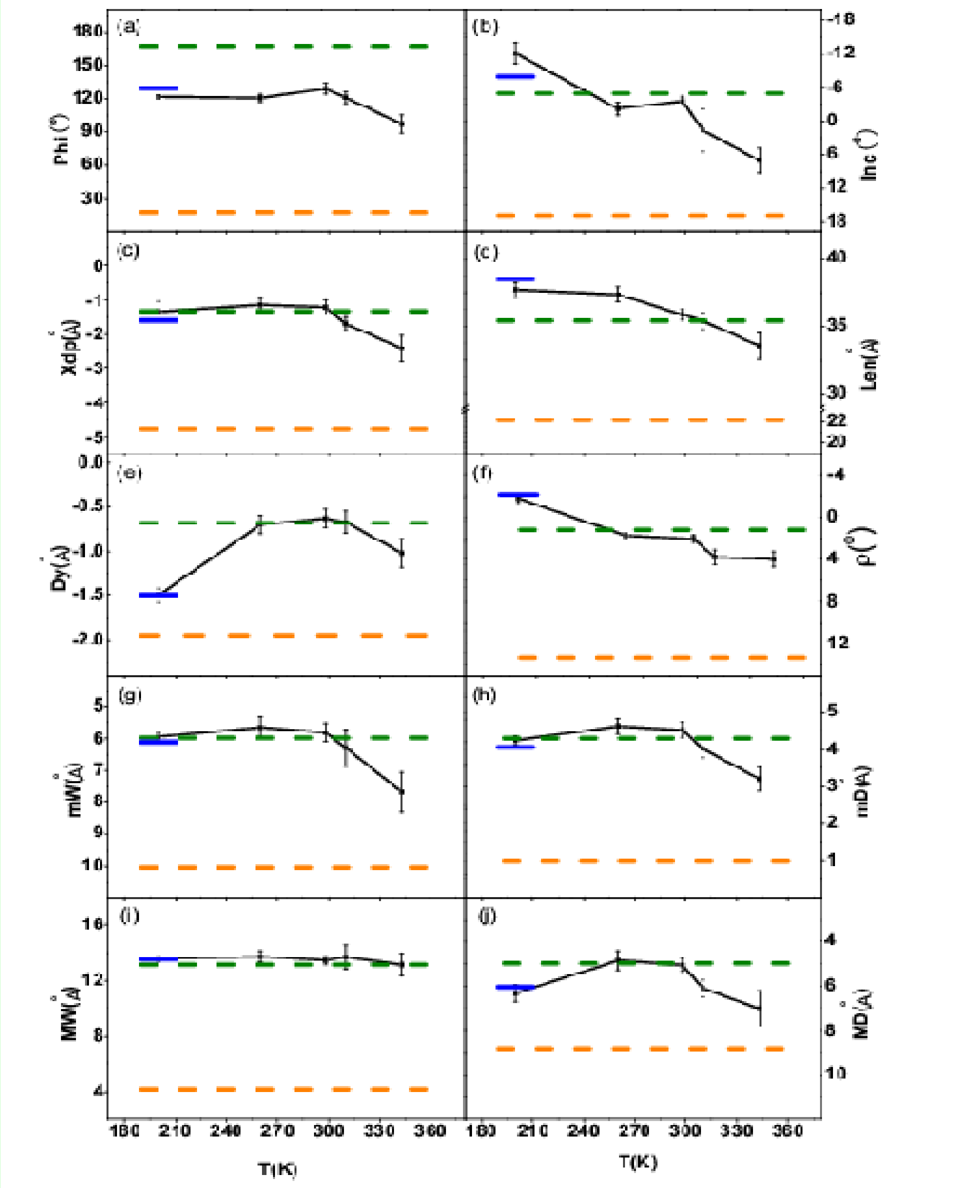
X. Shen,[1,2] B. Gu,[3] S. A. Che,[4] and F. S. Zhang[1,2,5,a)]
[1]*The Key Laboratory of Beam Technology and Material Modification of Ministry of Education, College of Nuclear Science and Technology, Beijing Normal University, Beijing 100875, China*
[2]*Beijing Radiation Center, Beijing 100875, China*
[3]*College of Math and Physics, Nanjing University of Information Science and Technology, Nanjing 210044, China*
[4]*School of Chemistry and Chemical Technology, Shanghai Jiao Tong University, Shanghai 200240, China*
[5]*Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator of Lanzhou, Lanzhou 730000, China*

(Received 11 December 2010; accepted 24 June 2011;

Counterions effects



Temperature effects



With the temperature rises, DNA structure changes to (A-B) Mix-DNA

Li^+、K^+、Rb^+、Cs^+ induced DNA conformation changes

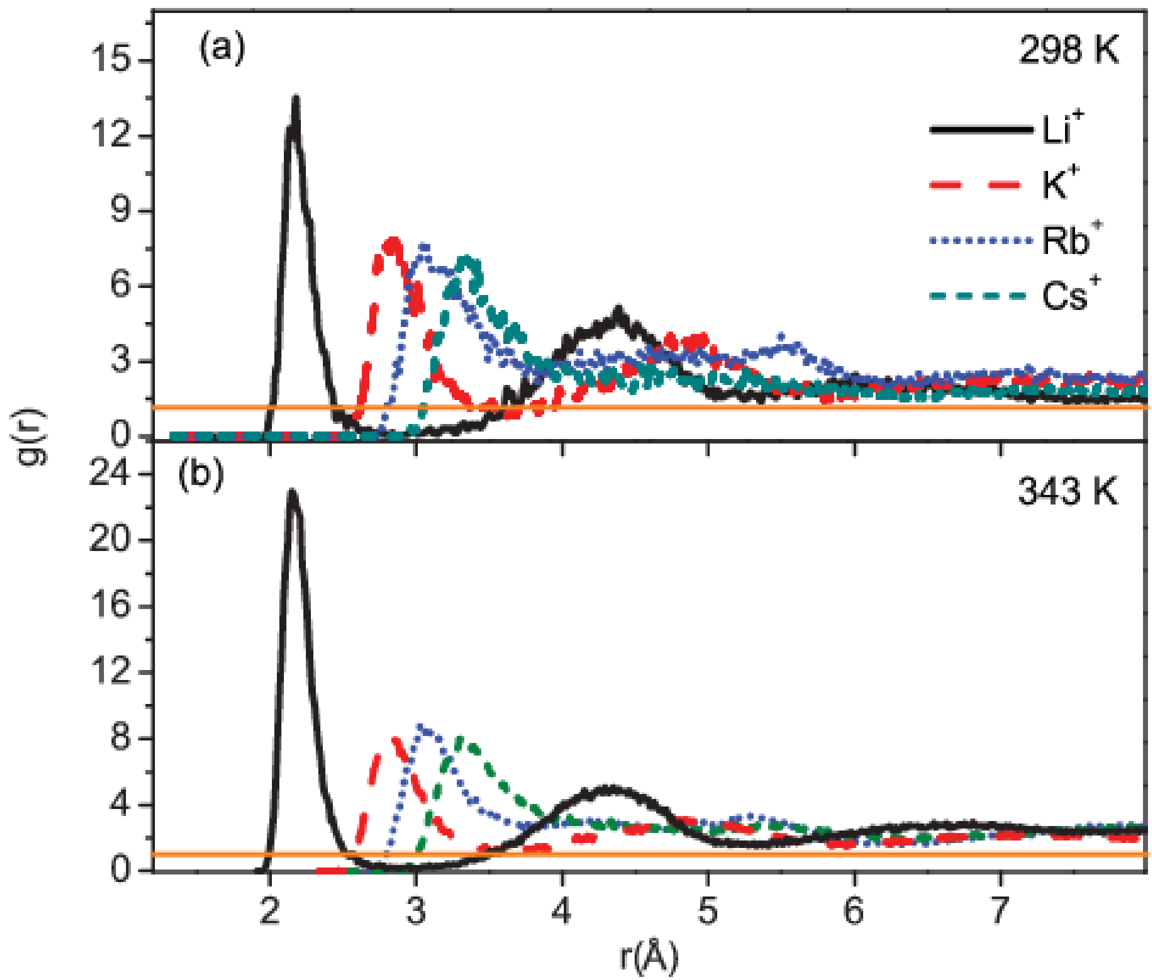
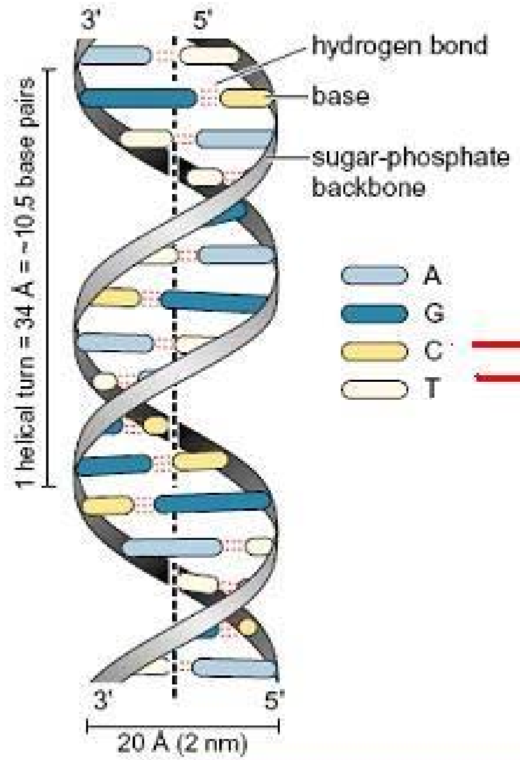


FIG. 8. RDFs of four ions around free phosphate oxygen atoms on the DNA backbones at two temperature. (a) ions-O^--(P) at 298 K. (b) ions-O^--(P) at 343 K.

Outline

1. Introduction
2. Applications
    2.1 Cancer therapy
    2.2 Seed breeding
    2.3 Space radiation
    2.4 Problems
3. A Multi-scale microscopic dynamical model
4. **Conclusions**



New Structure !

Physical process(10^{-24}~10^{-8}s) ⇒ Chemical process(10^{-8}s) ⇒ Biological process (10^{3}s)

Nuclear process (10^{-24}~10^{-18}s) ⇒ Electronic process (10^{-18}~10^{-12}s) ⇒ Relaxation process (10^{-12}~10^{-8}s)

Conclusions

- A preliminary version of:

A multi-scale microscopic dynamic approach to study interaction of heavy ions with biomolecules

- Smooth connections between different processes
  Nucl. → Elec. → Relax. → Micro-dose

- Relationship between the structures and biological functions of biomolecules

- Your ideas, suggestions, comments ?

Collaborators:

X. Shen, J. Su, B. Gu，Z.P. Wang，H.Y. Zhou

Discussions:

Y. Su, T. Zhang, H.Z. Shang, J.H. Zhang, N. Y. Wang, CNST-BNU
G. F. Zhang, School of Life Sciences-BNU

W.J. Li, Z.G. Wang, H. Zhang, G.M. Jin, G.Q. Xiao, IMP-CAS
Z.Y. Zhu, Z. Y. Zhu, L. Yan, SINAP-CAS
Y.Z. Zhuo, K. Zhao, CIAE

B.A. Li, tamu-commerce-USA
Y.W. Zhang, ORNL-USA
P.M. Dinh, E. Suraud, Paul Sabatier University-France
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5. Beijing Beijing Radiation Center
6. Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator of Lanzhou

Thank you for your attention !