From fundamental physics to the origins of life: ab initio Miller experiments

JE SUIS CHARLIE

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Osservatorio Astronomico – Trieste, February 18th 2015

SORBONNE UNIVERSITÉS

dépasser les frontières

Outline

- Origins of life: from Aristotle to Miller experiments

- The physicist's approach: from complex organisms to electronic wave-functions, and back ?

- *Ab initio* prebiotic chemistry and *in silico* Miller experiments

- Perspectives and conclusions

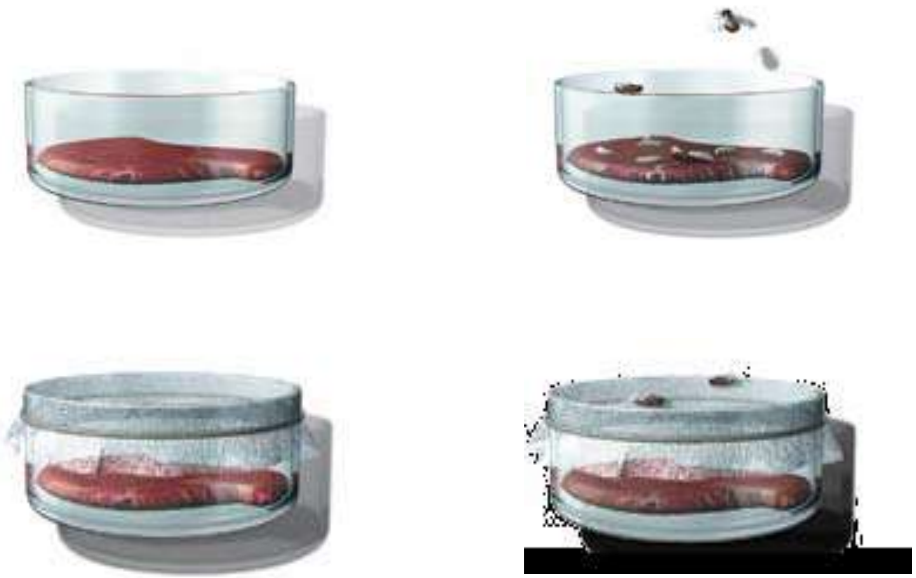
Origins of life: (a)biogenesis ?

- Aristotle's abiogenesis: life originating from non-living matter

Ancient & Middle Ages

Origins of life: (a)biogenesis ?

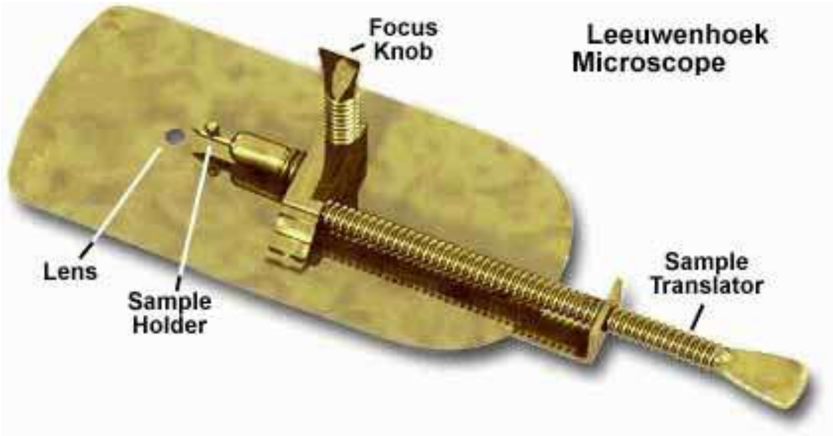
- ❑ Aristotle's abiogenesis: life originating from non-living matter
- ❑ Redi: the scientific method & biogenesis



Ancient & Middle Ages	1600's							

Origins of life: (a)biogenesis ?

- ❑ Aristotle's abiogenesis: life originating from non-living matter
- ❑ Redi: the scientific method & biogenesis
- ❑ Van Leewenhoek: microscope & abiogenesis



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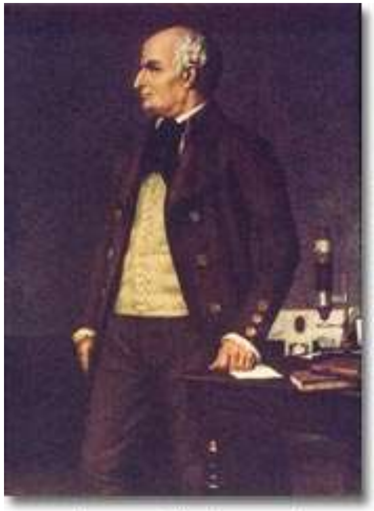
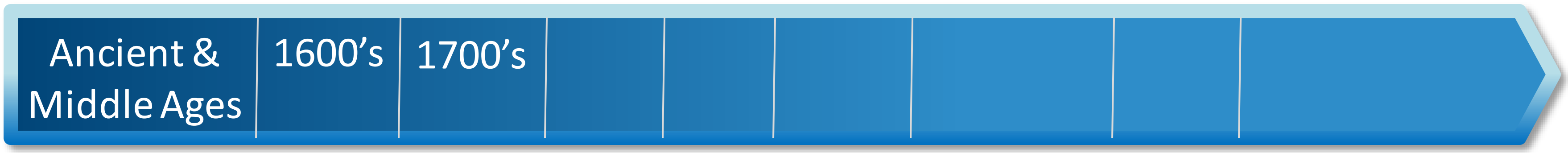
- ❑ Needham vs. Spallanzani



Lazzaro Spallanzani



Origins of life: (a)biogenesis ?

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- ❑ Redi: the scientific method & biogenesis
- ❑ Van Leewenhoek: microscope & abiogenesis

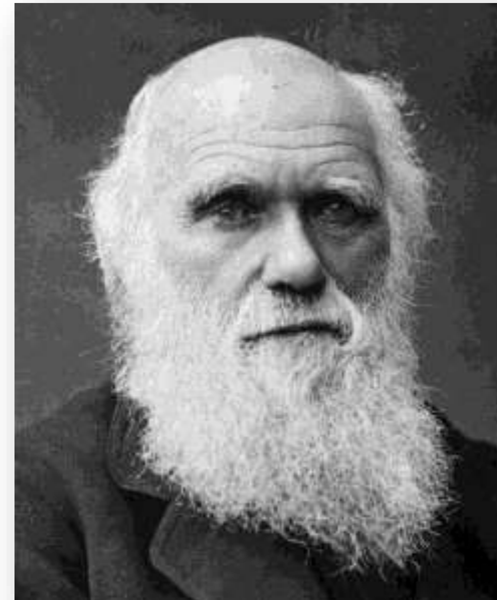
- ❑ Needham vs. Spallanzani

- ❑ Pasteur wins the Alhumbert prize <u>against abiogenesis</u>

Ancient & Middle Ages	1600’s	1700’s	1862					

Origins of life & modern theories

❑ Darwin, evolution, and the “warm little pond”



Ancient & Middle Ages	1600’s	1700’s	1862	1871				

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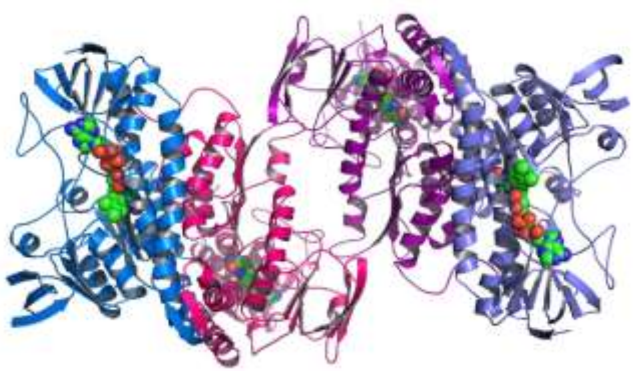
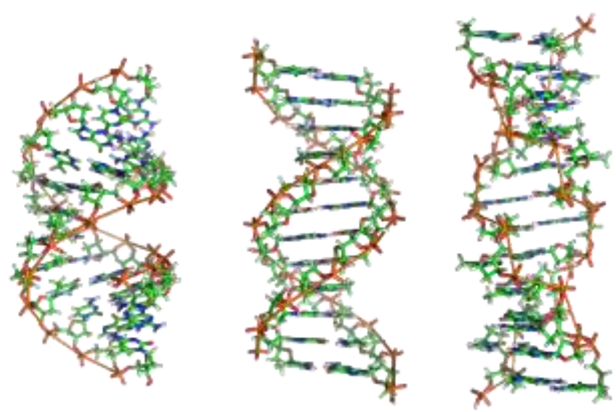
Ancient & Middle Ages	1600's	1700's	1862	1871				

Origins of life & modern theories

- Darwin, evolution, and the "warm little pond"

- Oparin and Haldane: hypothesis of <u>chemical</u> evolution





Ancient & Middle Ages	1600's	1700's	1862	1871	1920's			

Origins of life & modern theories

- ❑ Darwin, evolution, and the "warm little pond"
- ❑ Oparin and Haldane: hypothesis of chemical evolution
- ❑ Bernal defends Oparin's theories…

THE PROCEEDINGS OF THE PHYSICAL SOCIETY

Section B

VOL. 62, PART 10 — 1 October 1949 — No. 358 B

The Physical Basis of Life*

BY J. D. BERNAL†

Birkbeck College, London

32nd Guthrie Lecture, delivered 21st November 1947; MS. received 18th May 1949

Ancient & Middle Ages	1600's	1700's	1862	1871	1920's	Post-WWII		

Origins of life & modern theories

- Darwin, evolution, and the "warm little pond"
- Oparin and Haldane: hypothesis of chemical evolution
- Bernal defends Oparin's theories
- … and Urey begins to look into it

ON THE EARLY CHEMICAL HISTORY OF THE EARTH AND THE ORIGIN OF LIFE

BY HAROLD C. UREY

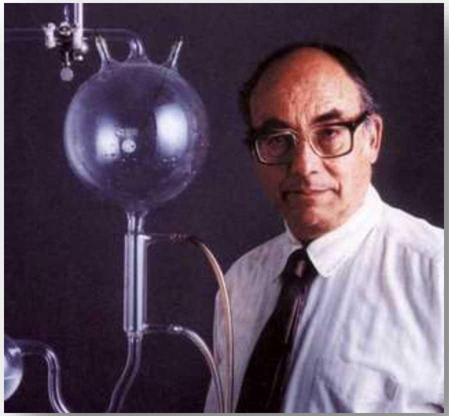
INSTITUTE FOR NUCLEAR STUDIES, UNIVERSITY OF CHICAGO

Communicated January 26, 1952

Ancient & Middle Ages	1600's	1700's	1862	1871	1920's	Post-WWII		

Miller(-Urey) experiment(s)

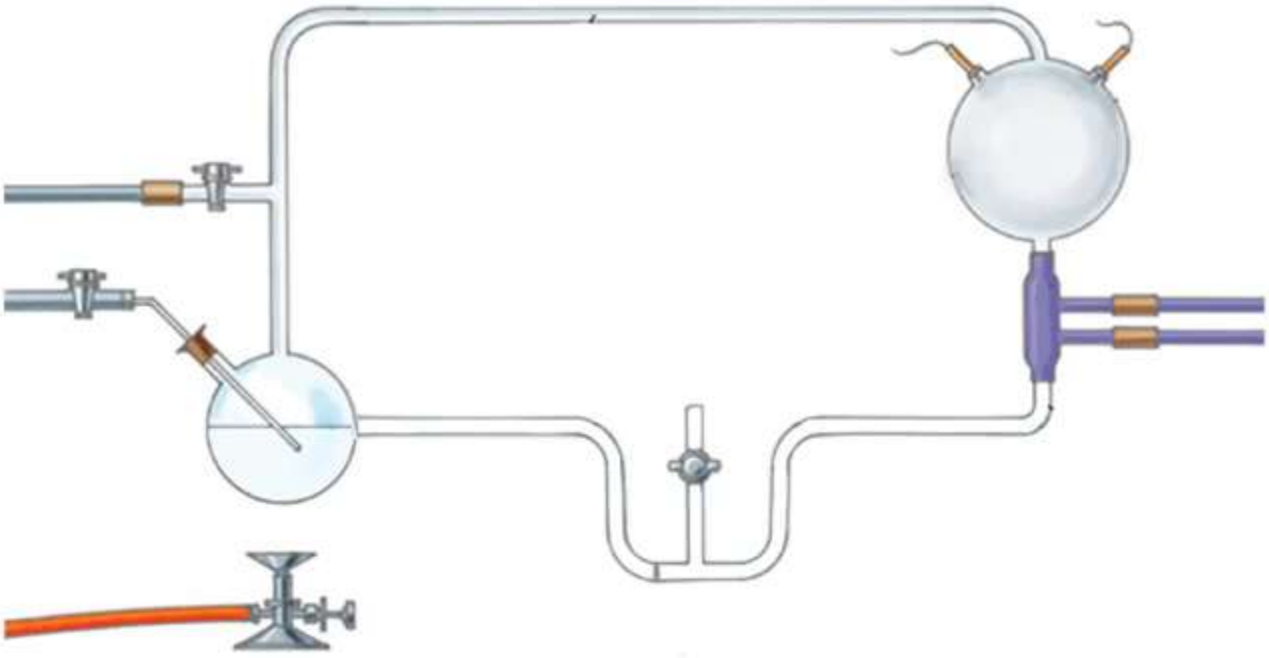
- 1950's: hypotheses on early Earth atmosphere and conditions
- Strong volcanic activities, lightning
- Reducing chemical composition: H_2O, NH_3, CH_4, H_2

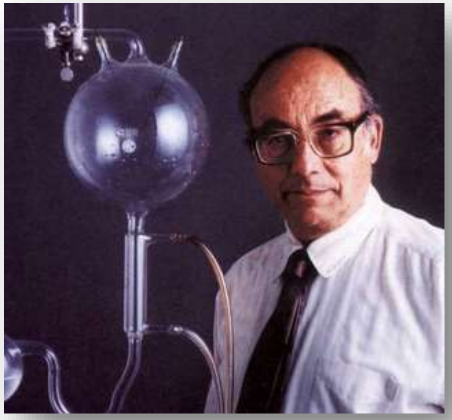


Ancient & Middle Ages	1600's	1700's	1862	1871	1920's	Post-WWII	1953	

Miller(-Urey) experiment(s)

- 1953: Milestone lab simulation of lightning in primordial atmosphere





Ancient & Middle Ages	1600's	1700's	1862	1871	1920's	Post-WWII	1953	

Miller's breakthrough

- Single event redefining the "origins of life" research

- Repeated over the decades with more realistic (oxidizing) atmospheres, including H_2S, CO_2 ,CO

- Juan Oró (1960): synthesis of nucleic acids bases from HCN solutions

- Synthesis of elementary biological monomers from simple molecules: prebiotic chemistry is born

Ancient & Middle Ages	1600's	1700's	1862	1871	1920's	Post-WWII	1953	Modern research

Aftermath of Miller's experiment: moving up the ladder of complexity

1. From simple "Miller" molecules to biological monomers

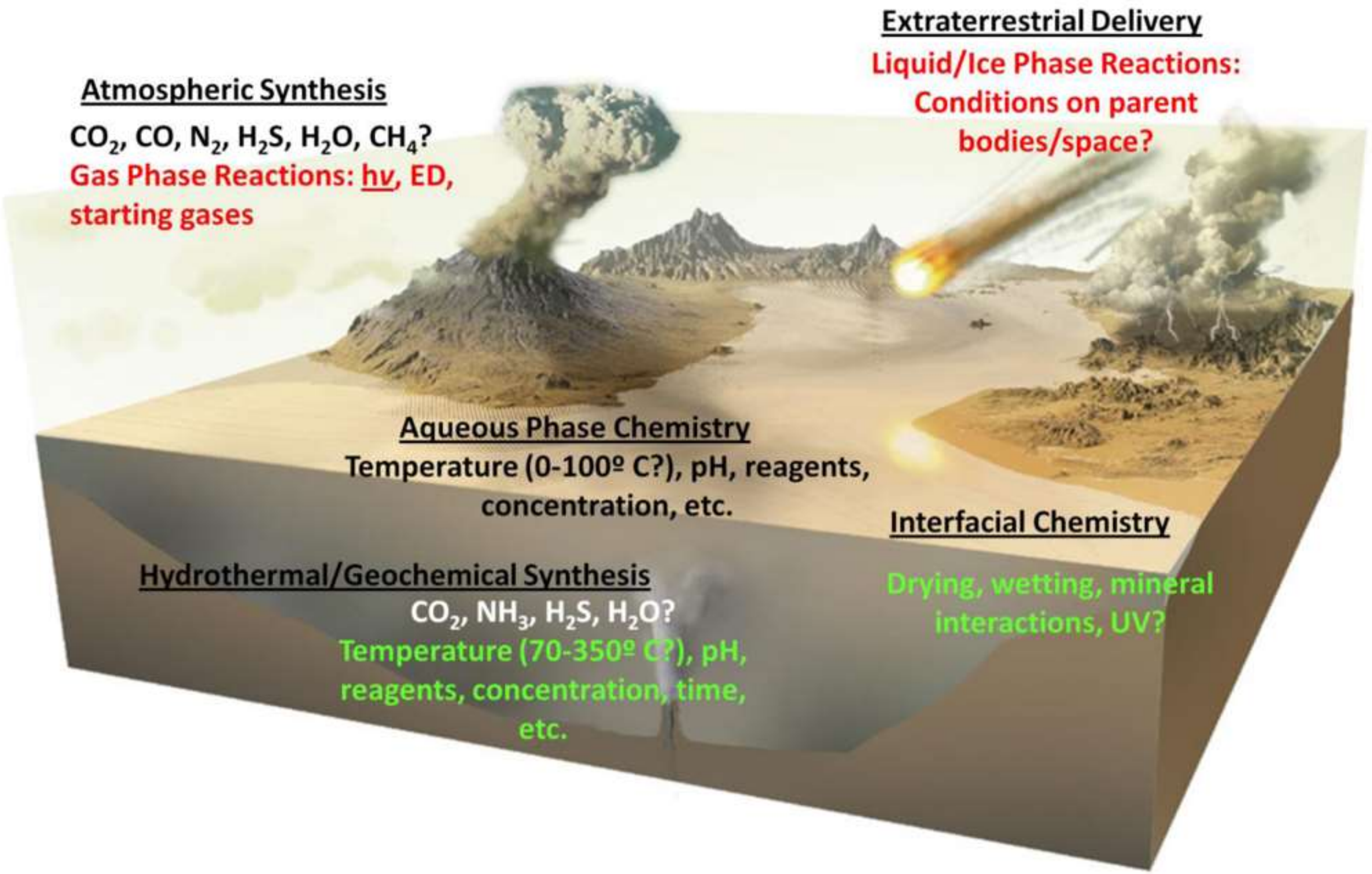
2. …to biological polymers (proteins, nucleic acids, etc…)

3. …to self-replication and hereditarity, "protein world" vs "RNA world"

4. …to organelles, cells, microscopic, and macroscopic life

Ancient & Middle Ages	1600's	1700's	1862	1871	1920's	Post-WWII	1953	Modern research

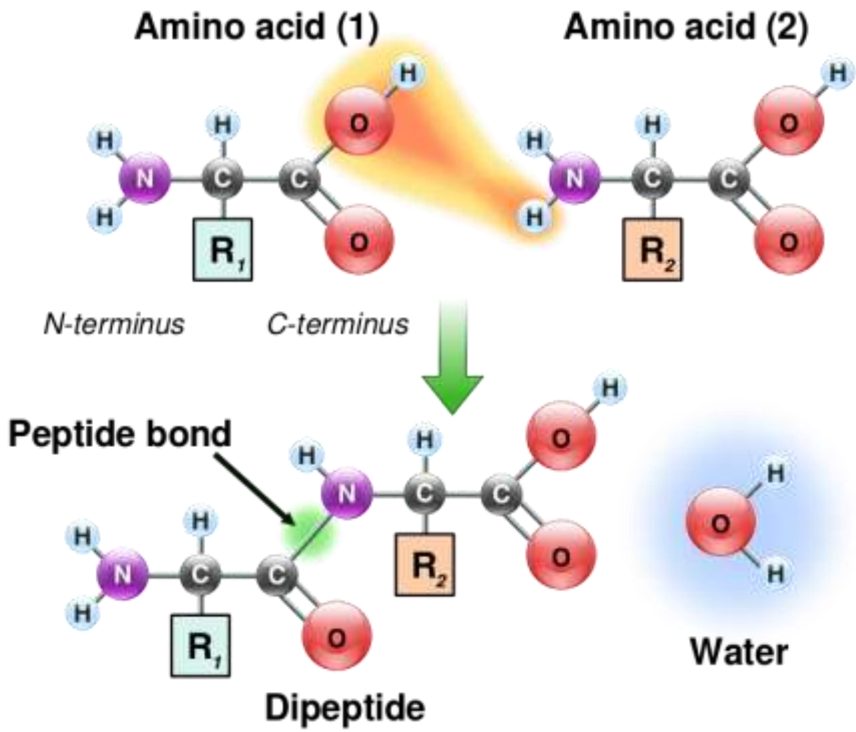
Aftermath of Miller's experiment: other potential sources of chemical energy?



Ancient & Middle Ages	1600's	1700's	1862	1871	1920's	Post-WWII	1953	Modern research

Aftermath of Miller's experiment: the emergence of complexity?

- From biological monomers to polymers? Unfavored in solution!



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Aftermath of Miller's experiment: the emergence of complexity?

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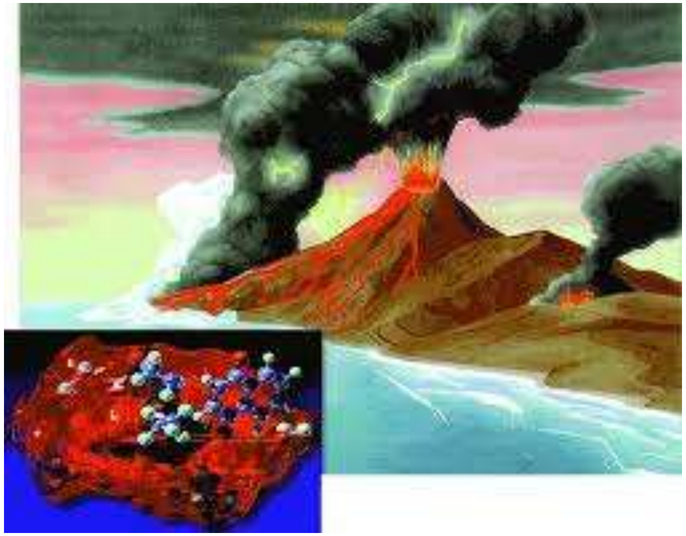
- Fox & Harada "Miller experiment" (1964) in ultra-dry conditions



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Aftermath of Miller's experiment: the emergence of complexity?

- ❑ From biological monomers to polymers? Unfavored in solution!

- ❑ Fox & Harada "Miller experiment" (1964) in ultra-dry conditions

- ❑ "Polymerization on the rocks" (Bernal, 1961)

Ancient & Middle Ages	1600's	1700's	1862	1871	1920's	Post-WWII	1953	Modern research

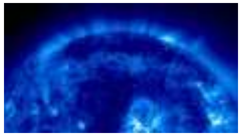
Origins of life?

- ❑ Extraterrestrial: life building-blocks arrived from the sky

- ❑ Meteoritic: extreme pressures and temperatures from bolide impacts

- ❑ Submarine: hydrothermal conditions in oceanic vents

- ❑ Ultra-violet: UV sunlight-induced prebiotic synthesis

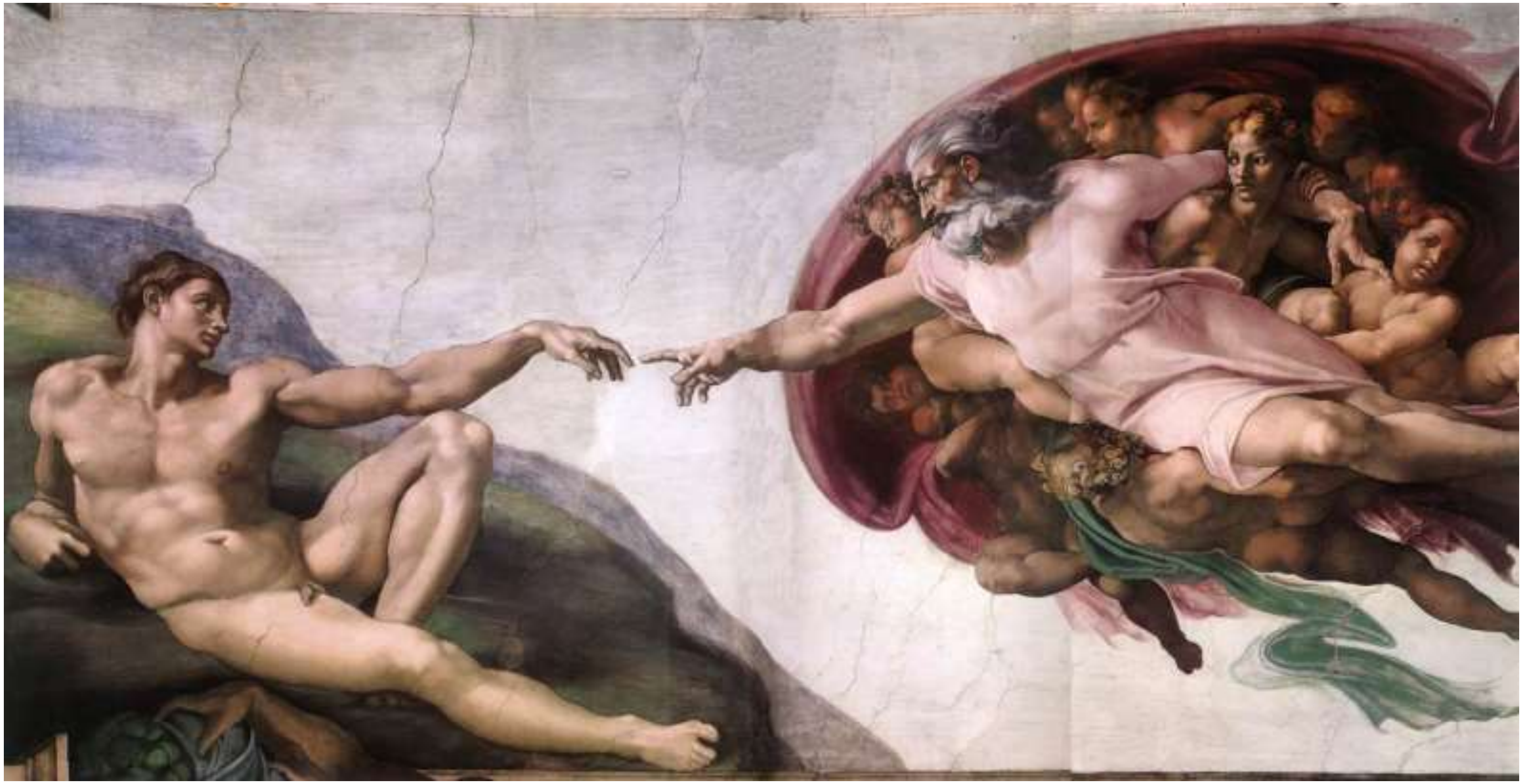


- ❑ Iron-sulphur world: synthesis at the mineral surface

Ancient & Middle Ages	1600's	1700's	1862	1871	1920's	Post-WWII	1953	Modern research

WHY ARE WE HERE?

Why are we here?



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- ❑ Origins of life: from Aristotle to Miller experiments

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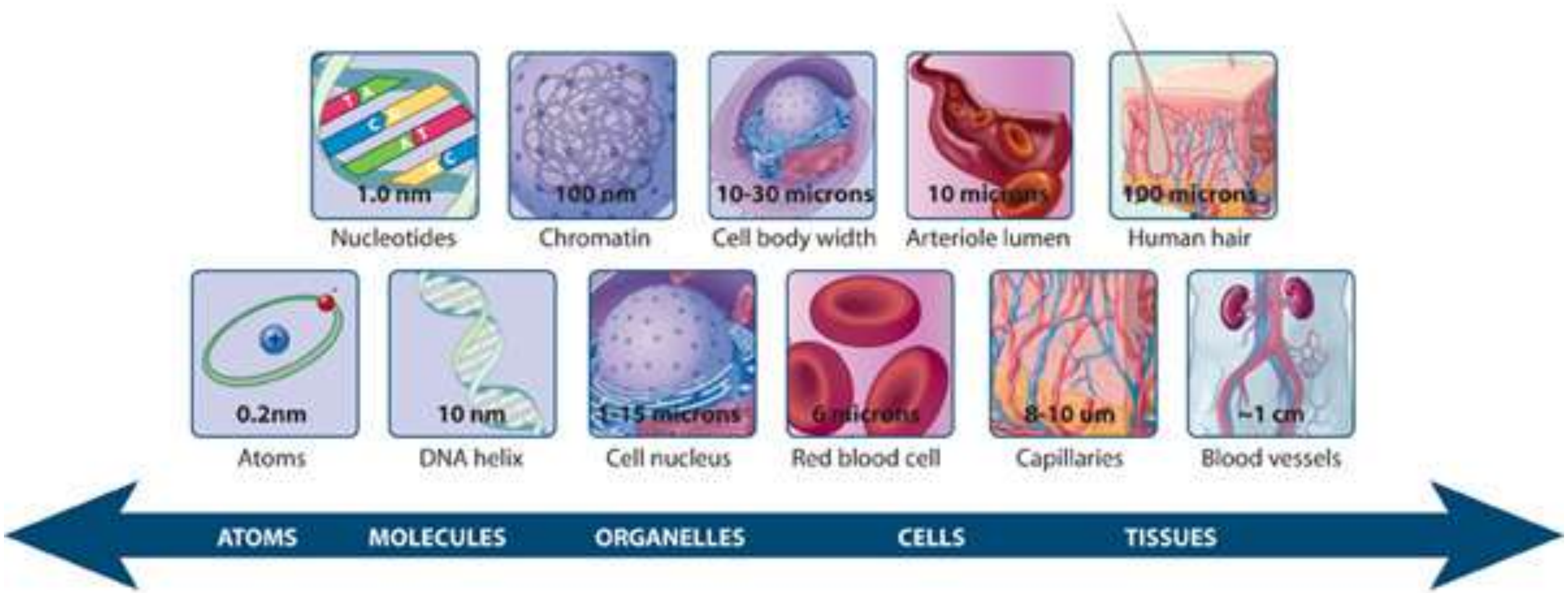
- ❑ *Ab initio* prebiotic chemistry and *in silico* Miller experiments

- ❑ Perspectives and conclusions

Why are we here?

- **Miller's experiment**: philosophy, biology, Earth science, chemistry… physics?

- 2014: can we retrace it, step by step, starting from fundamental physics laws?



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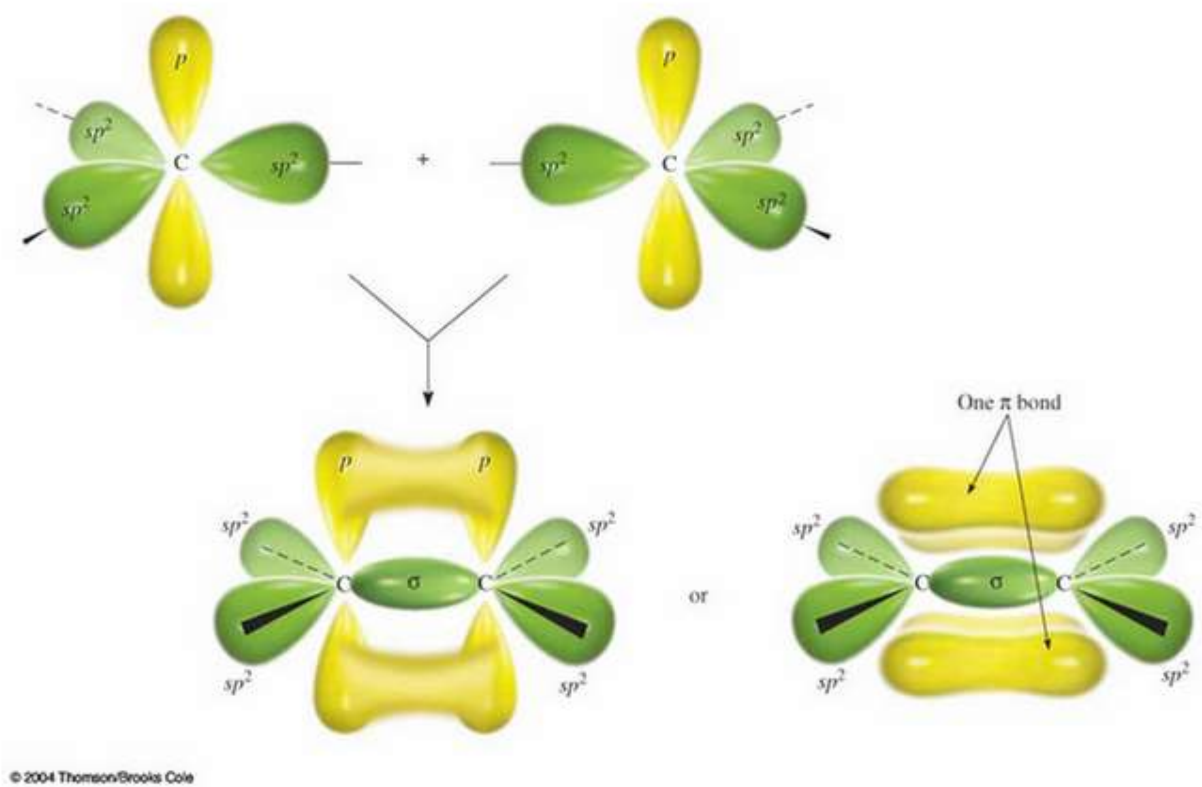


What causes “Miller” prebiotic reactions?

- ❑ External energy/temperature?
- ❑ Ionization?
- ❑ Electric field?

Why are we here?

- Miller's experiment: philosophy, biology, Earth science, chemistry… physics?

- 2014: can we retrace it, step by step, starting from fundamental physics laws?

  1. Solve the many-body Schrödinger equation

  2. Finite-temperature exploration of phase and reaction space

  3. Apply an external electric field?

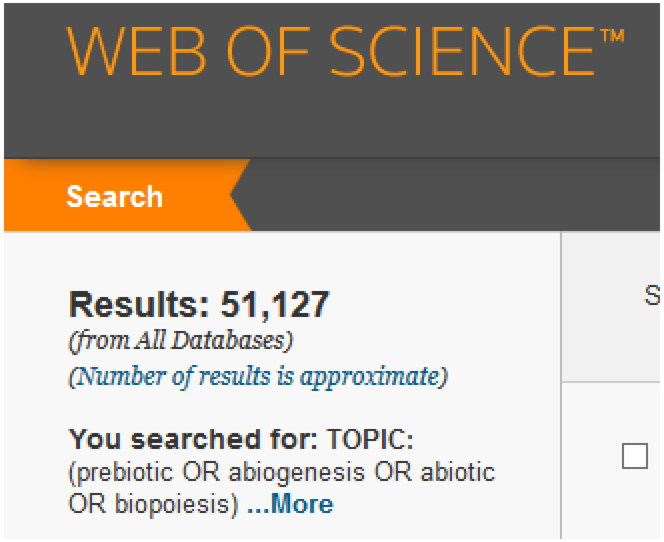
Ab initio calculations

- Many-electron problem: Slater, Hartree, Hartree-Fock

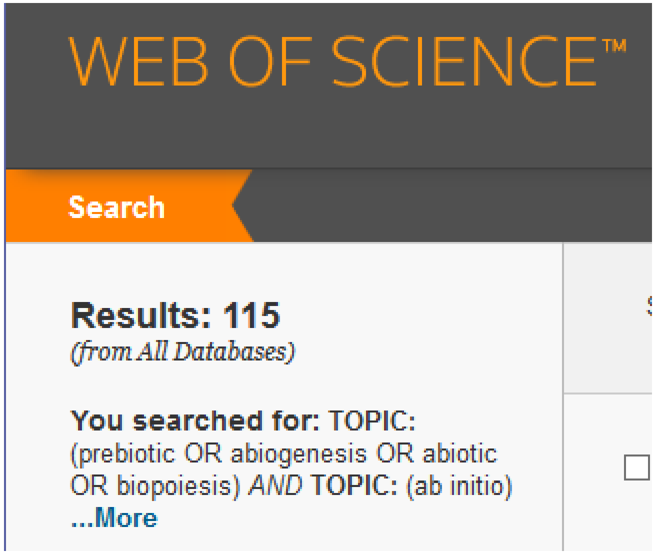
- Quantum chemistry: Møller-Plesset, Configuration-Interaction, Coupled-Cluster…

Ab initio prebiotic chemistry?

- « Prebiotic » : 50,000+ hits



- « Ab initio » AND « Prebiotic » : 115 hits



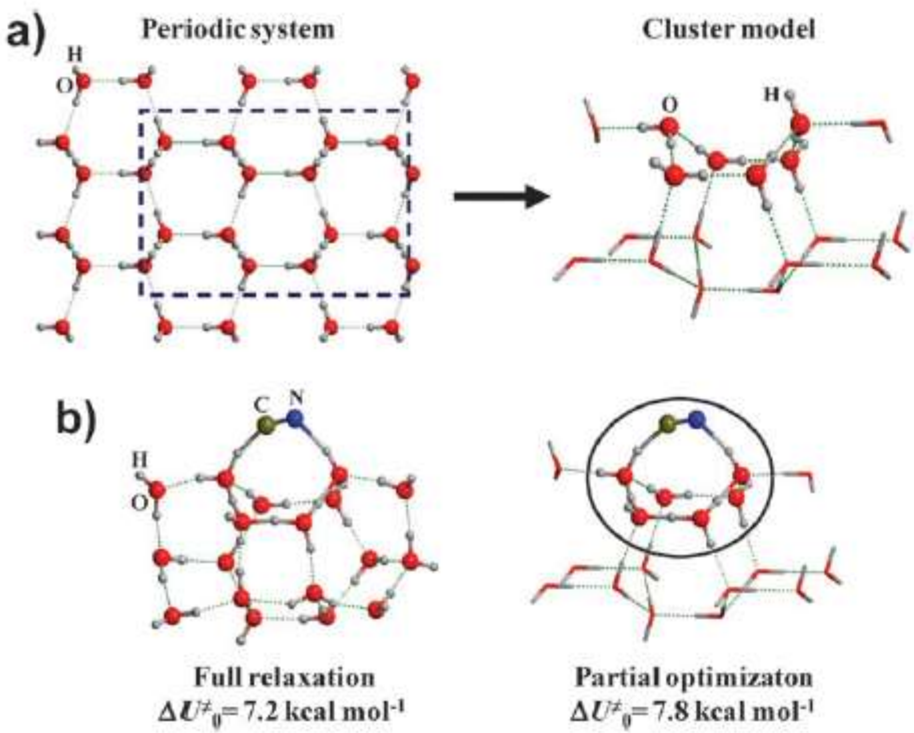
Ab initio prebiotic chemistry

PAPER www.rsc.org/pccp | Physical Chemistry Chemical Physics

Deep-space glycine formation *via* Strecker-type reactions activated by ice water dust mantles. A computational approach†

Albert Rimola,[a] Mariona Sodupe*[b] and Piero Ugliengo*[a]

Received 9th November 2009, Accepted 17th February 2010
First published as an Advance Article on the web 31st March 2010

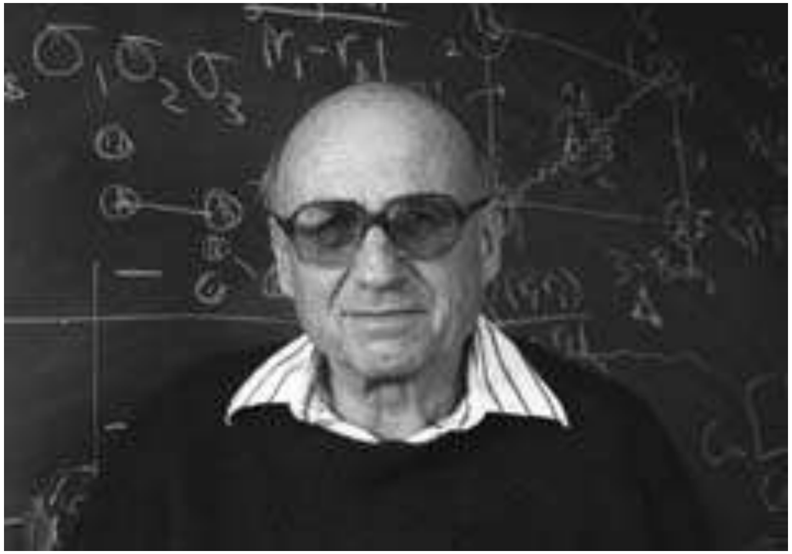


Ab initio-DFT calculations

- ❑ Many-electron problem: Slater, Hartree, Hartree-Fock

- ❑ Quantum chemistry: Møller-Plesset, Configuration-Interaction, Coupled-Cluster…

- ❑ Density-Functional Theory (DFT)



Ab initio-DFT calculations

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- Density-Functional Theory (DFT)

$$E[n] = T_s[n] + \int d^3r\, V_{\mathrm{ext}}(\vec{r})\, n(\vec{r}) + E_{\mathrm{H}}[n] + E_{\mathrm{xc}}[n]$$

$$\left[-\frac{\hbar^2 \nabla_2}{2m} + V_{\mathrm{ext}}(\vec{r}) + e^2 \int d^3r' \frac{n(\vec{r'})}{|\vec{r} - \vec{r'}|} + V_{\mathrm{xc}}(\vec{r};[n])\right] \psi_j(\vec{r}) = \varepsilon_j \psi_j(\vec{r})$$

$$n(\vec{r}) = \sum_j f_j \mid \psi_j(\vec{r}) \mid^2$$

Why are we here?

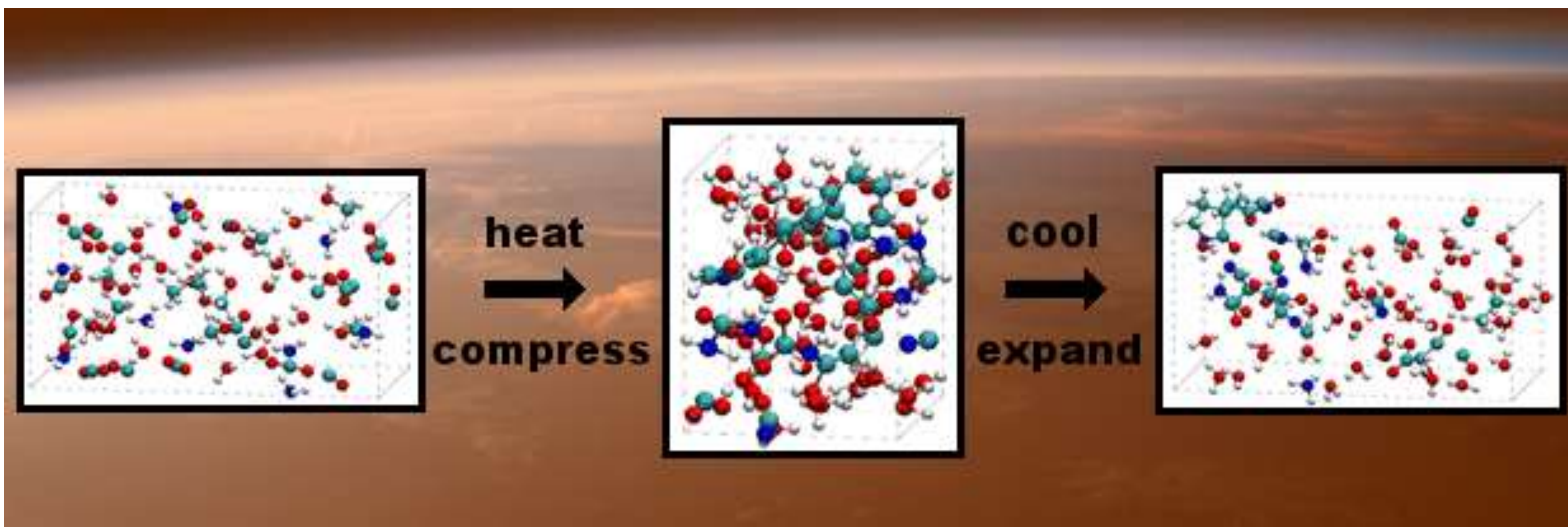
- Miller's experiment: philosophy, biology, Earth science, chemistry… physics?
- 2014: can we retrace it, step by step, starting from fundamental physics laws?
    - Many-body Schrödinger equation: Density Functional Theory (1963) (W. Kohn, Nobel 1998)
    - Finite temperature: Ab Initio Molecular Dynamics (1985) (R. Car & M. Parrinello)

Ab initio prebiotic chemistry

nature chemistry
ARTICLES
PUBLISHED ONLINE: 12 SEPTEMBER 2010 | DOI: 10.1038/NCHEM.827

Synthesis of glycine-containing complexes in impacts of comets on early Earth

Nir Goldman*, Evan J. Reed†, Laurence E. Fried, I.-F. William Kuo and Amitesh Maiti



Ab initio prebiotic chemistry

JACS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ARTICLE

pubs.acs.org/JACS

Peptide Synthesis in Aqueous Environments: The Role of Extreme Conditions and Pyrite Mineral Surfaces on Formation and Hydrolysis of Peptides

Eduard Schreiner,*,† Nisanth N. Nair,‡ Carsten Wittekindt, and Dominik Marx

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  - Many-body Schrödinger equation: Density Functional Theory (1963) (W. Kohn, Nobel 1998)
  - Finite temperature: Ab Initio Molecular Dynamics (1985) (R. Car & M. Parrinello)
  - Apply an external electric field?

Electric field in ab initio calculations ?

- Density-Functional Theory (DFT)

$$\left[-\frac{\hbar^2 \nabla_2}{2m} + V_{\rm ext}(\vec{r}) + e^2 \int d^3r' \, \frac{n(\vec{r'})}{|\vec{r}-\vec{r'}|} + V_{\rm xc}(\vec{r};[n])\right] \psi_j(\vec{r}) = \varepsilon_j \psi_j(\vec{r})$$

$$n(\vec{r}) = \sum_j f_j \; | \, \psi_j(\vec{r}) \, |^2$$

- Plane-wave expansion

$$\psi_{m,\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N\Omega_0}} \, \mathrm{e}^{\mathrm{i}\,\vec{k}\cdot\vec{r}} u_{m,\vec{k}}(\vec{r})$$

$$u_{m,\vec{k}}(\vec{r}) = \sum_{\{\vec{G}\}} \mathrm{e}^{\mathrm{i}\,\vec{G}\cdot\vec{r}} \; \tilde{u}_m(\vec{k}+\vec{G})$$

Electric field in ab initio calculations ?

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$$\left[-\frac{\hbar^2 \nabla_2}{2m} + V_{\mathrm{ext}}(\vec{r}) + e^2 \int d^3r' \, \frac{n(\vec{r'})}{|\vec{r}-\vec{r'}|} + V_{\mathrm{xc}}(\vec{r};[n])\right] \psi_j(\vec{r}) = \varepsilon_j \psi_j(\vec{r})$$

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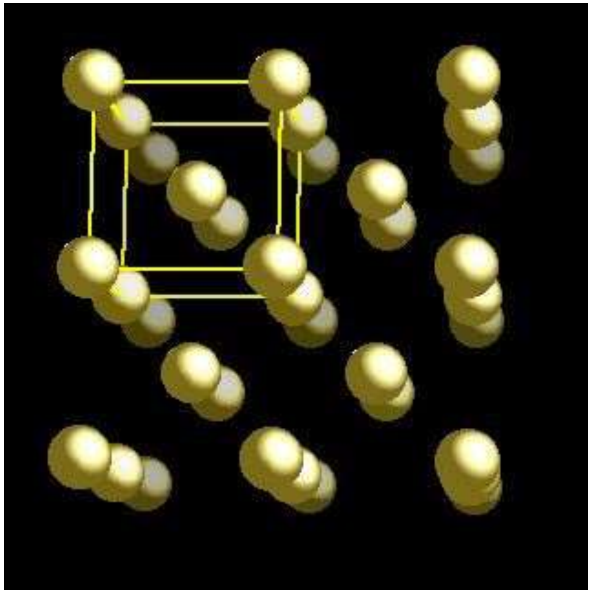
- Periodic Boundary Conditions (PBC)



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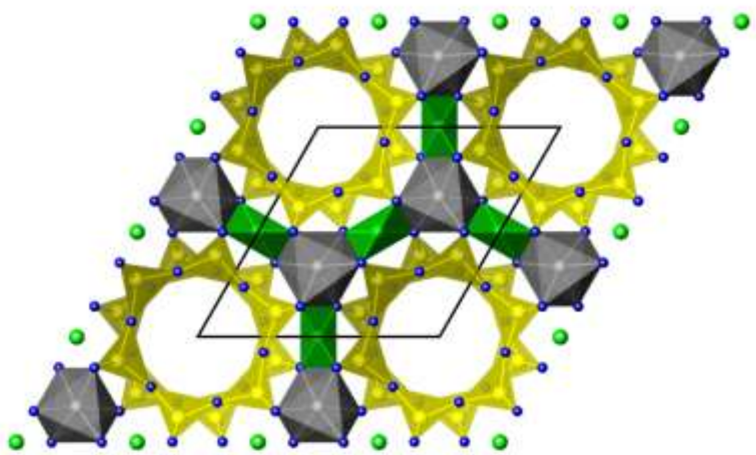
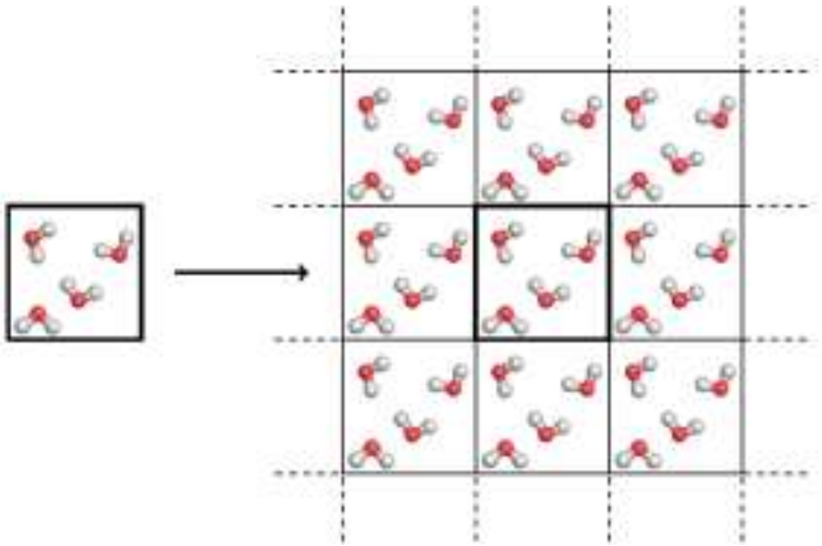


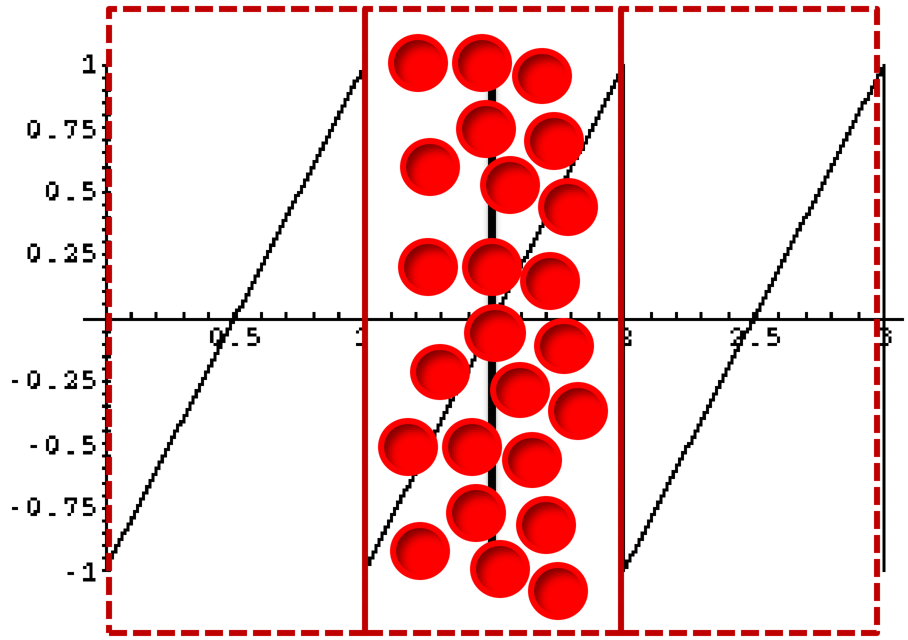


Electric field in ab initio calculations ?

- Periodic boundary conditions: sawtooth potential

- Low-D system: no problem

- Bulk system: unphysical !!



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  - Many-body Schrödinger equation: Density Functional Theory (1963) (W. Kohn, Nobel 1998)
  - Finite temperature: Ab Initio Molecular Dynamics (1985) (R. Car & M. Parrinello)
  - Electric field in quantum mechanics: Berry-phase theory of polarization (1983) (R. Resta, D. Vanderbilt, 1993)

Electric field in ab initio calculations ?

- ❑ Periodic boundary conditions: sawtooth potential
- ❑ Low-D system: no problem
- ❑ Bulk system: unphysical !!
- ❑ Berry-phase theory of polarization

$$E^{\mathcal{E}}[\{\psi_i\}] = E^{(0)}[\{\psi_i\}] - \mathcal{E} \cdot P[\{\psi_i\}],$$

$$P[\{\psi_i\}] = -\frac{L}{\pi} \operatorname{Im}(\ln \det S[\{\psi_i\}]),$$

$$S_{ij} = \langle \psi_i | e^{2\pi i x/L} | \psi_j \rangle.$$

$$\epsilon_\infty = \frac{4\pi}{L^3} \frac{\Delta P^{\mathcal{E}}}{\mathcal{E}} + 1,$$

VOLUME 89, NUMBER 15 PHYSICAL REVIEW LETTERS 7 OCTOBER 2002

Ab initio Molecular Dynamics in a Finite Homogeneous Electric Field

P. Umari and Alfredo Pasquarello

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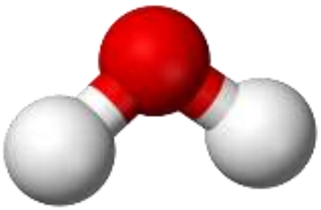
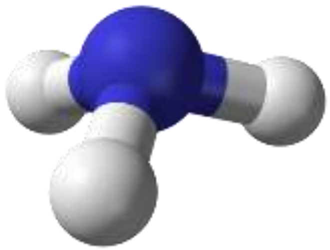
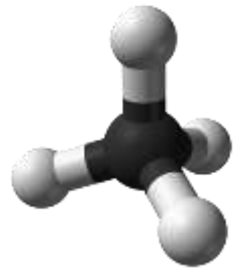
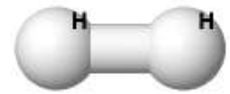
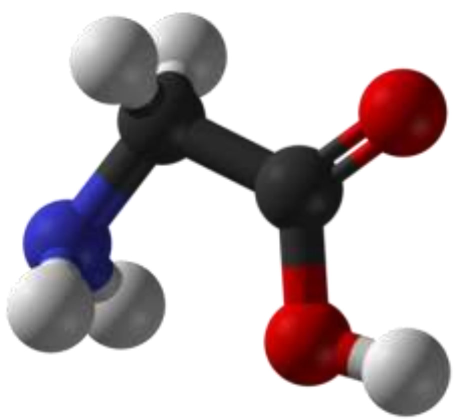
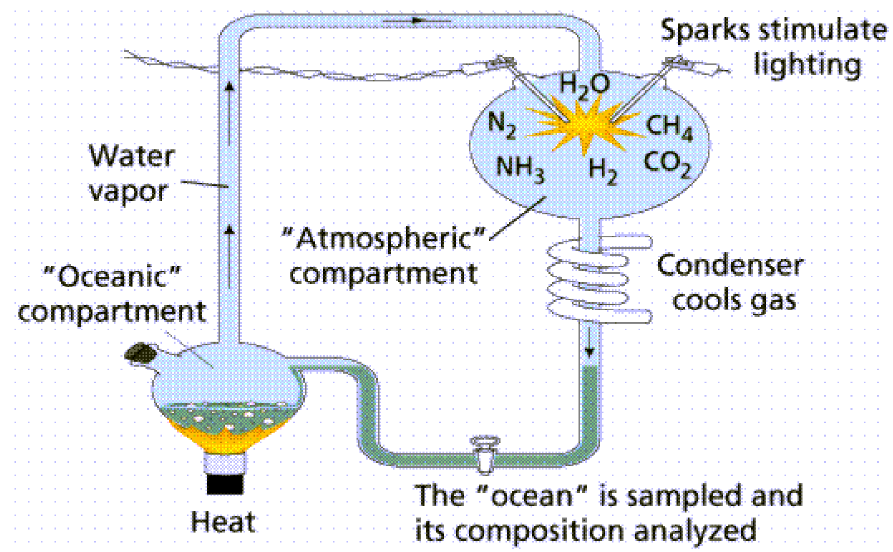
In silico Miller experiments?

- ❑ Start: simple molecules in aqueous environment

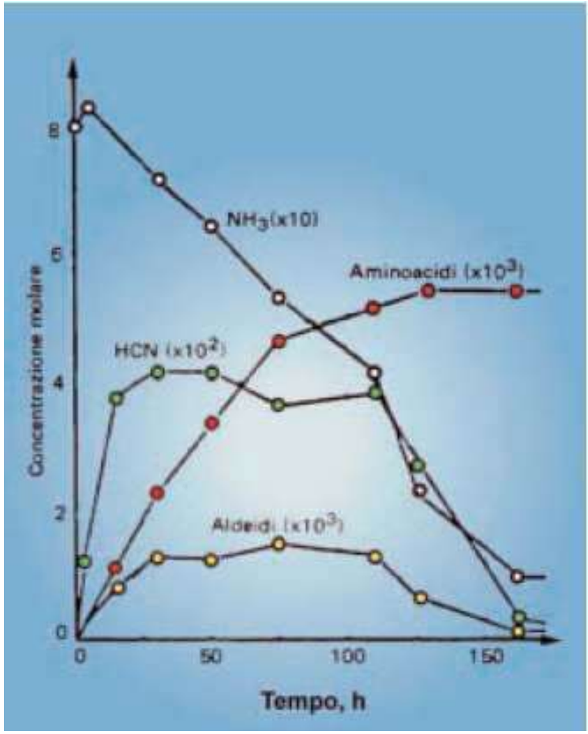





- ❑ End: glycine formation

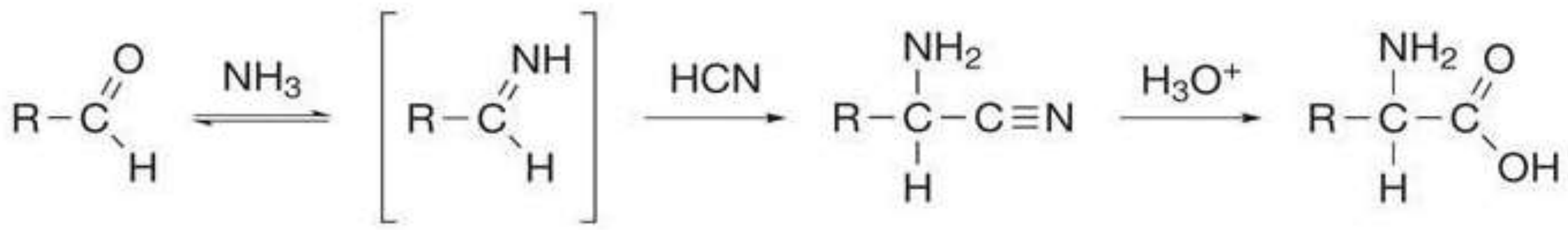



In silico Miller experiments?

- Aldehydes & HCN intermediate products



- Traditionally explained via Strecker reaction



In silico Miller experiments – I
Strecker reaction

- Intermediate steps: formaldehyde+HCN

$$CH_2O + HCN + NH_3 + H_2O \rightarrow NH_2\text{-}CH_2\text{-}CN + 2H_2O$$

$$NH_2\text{-}CH_2\text{-}CN + 2H_2O \rightarrow NH_3 + NH_2\text{-}CH_2\text{-}COOH$$

- Constant number of atoms in simulations: build up a supercell compatible with Strecker reaction?

- End and intermediate product, C:O:N:H = 1:1:1:4

AMS and F. Saija, PNAS 111, 13768 (2014)

In silico Miller experiments – I
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$$NH_2\text{-}CH_2\text{-}CN + 2H_2O \rightarrow NH_3 + NH_2\text{-}CH_2\text{-}COOH$$

Prebiotic synthesis from CO atmospheres: Implications for the origins of life

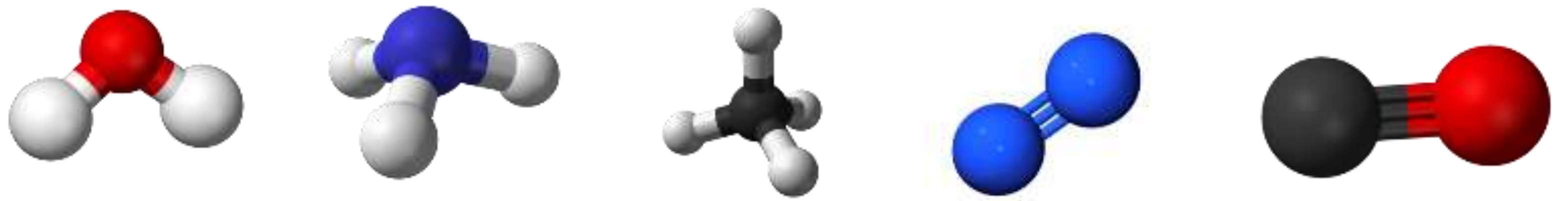
Shin Miyakawa*†, Hiroto Yamanashi*, Kensei Kobayashi*, H. James Cleaves‡, and Stanley L. Miller‡

*Department of Chemistry and Biotechnology, Faculty of Engineering, Yokohama National University, Yokohama 240-8501, Japan; and ‡Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA 92093-0506

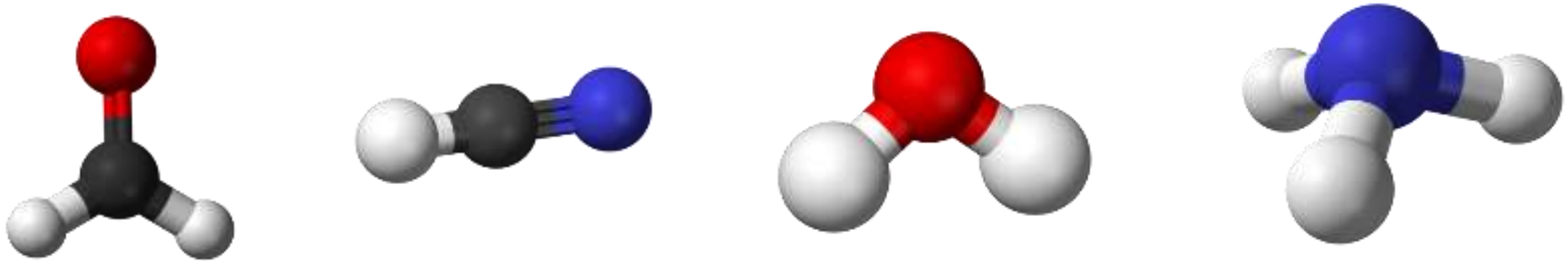
Contributed by Stanley L. Miller, September 19, 2002

In silico Miller experiments – II
Strecker reaction

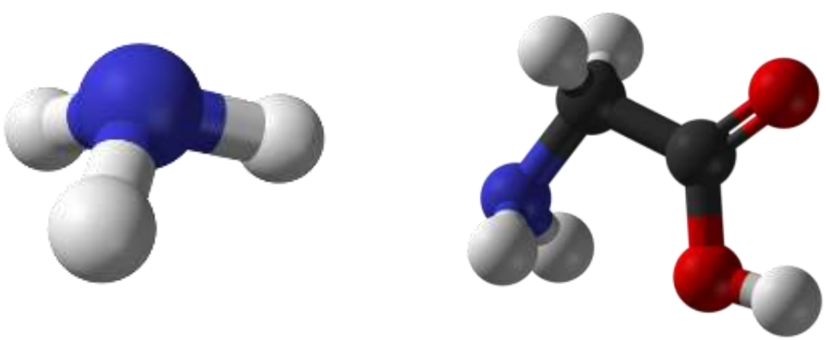
- Start mixture: 8 + 8 + 8 + 5 + 10 => C:O:N:H = 18:18:18:72



- Strecker intermediates: 9 + 9 + 9 + 9 => C:O:N:H = 18:18:18:72



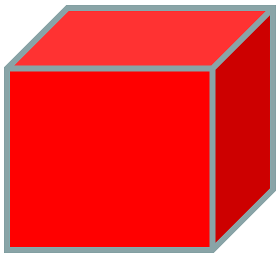
- Strecker products: 9 + 9 => C:O:N:H = 18:18:18:72



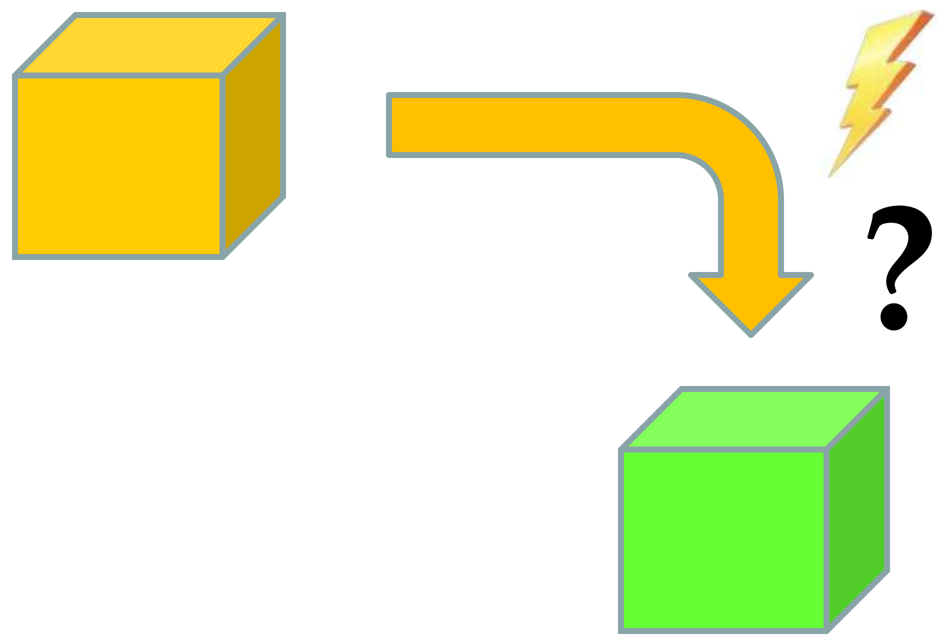
AMS and F. Saija, PNAS 111, 13768 (2014)

In silico Miller experiments – II
Strecker reaction

- Start mixture



- Strecker intermediates



- Strecker products

AMS and F. Saija, PNAS 111, 13768 (2014)

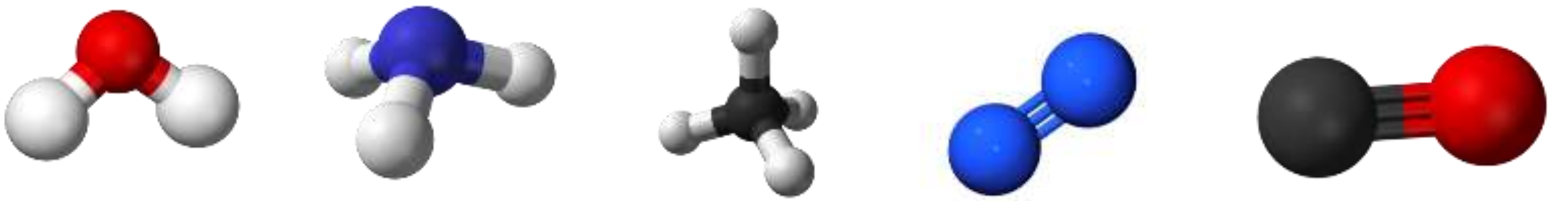
Computational details

- Density-Functional Theory – Ab Initio Molecular Dynamics
- Plane-wave/pseudopotential approach (Quantum-Espresso)
- 35 Ry cutoff/PBE US pseudopotentials
- ~40-50 molecules, 126-160 atoms, 20-50 ps trajectories
- 1.0 gr/mL density, T = 400 K
- Electric fields: 0.0 – 0.5 V/Å

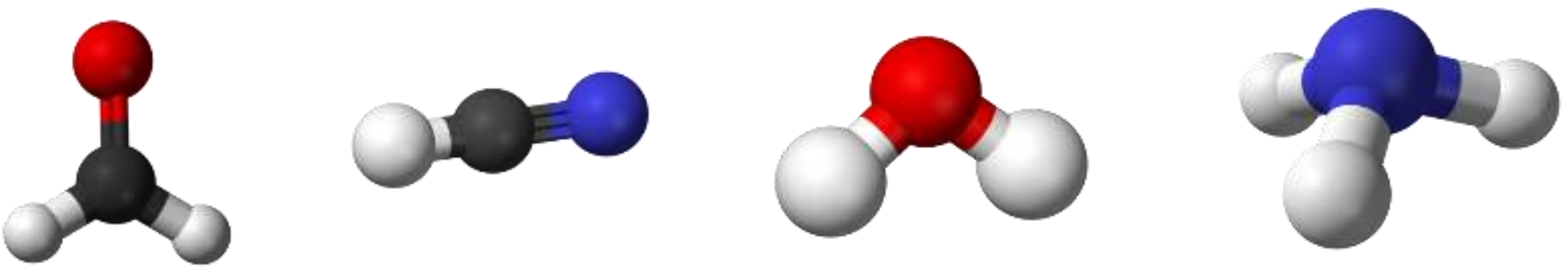
AMS and F. Saija, PNAS 111, 13768 (2014)

In silico Miller experiments – II Strecker reaction

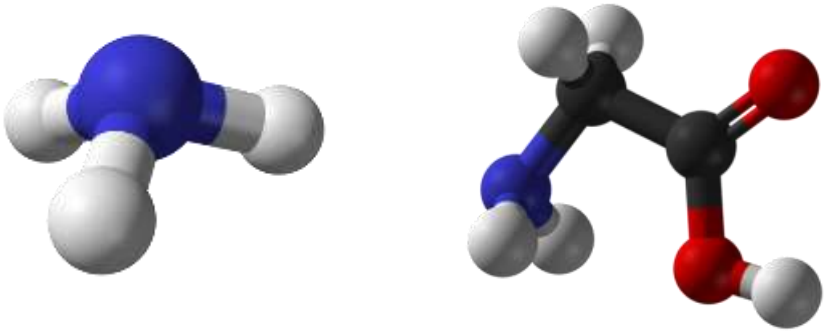
- Start: Miller molecules in zero field



- Strecker intermediate step in zero field: higher energy!!



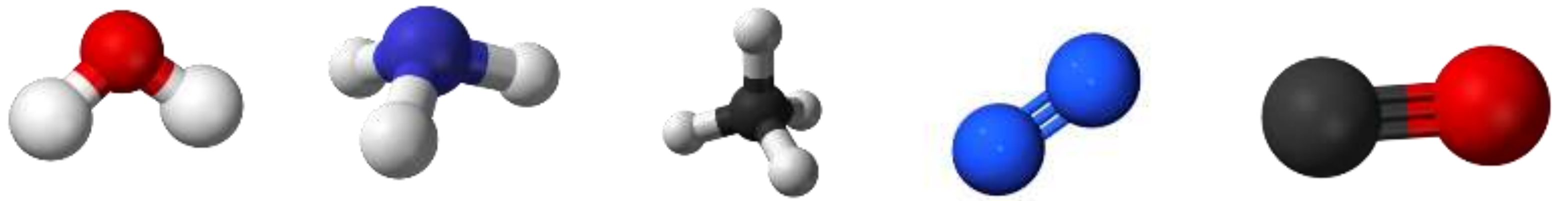
- Strecker final step: glycine and ammonia in zero field



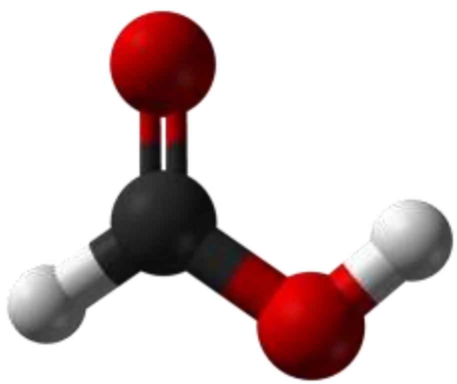
AMS and F. Saija, PNAS 111, 13768 (2014)

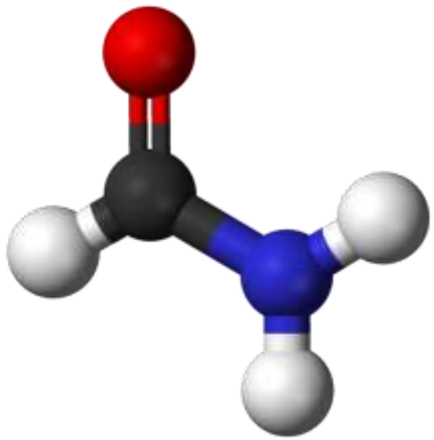
In silico Miller experiments – II
Strecker reaction

- Start: Miller molecules in strong fields



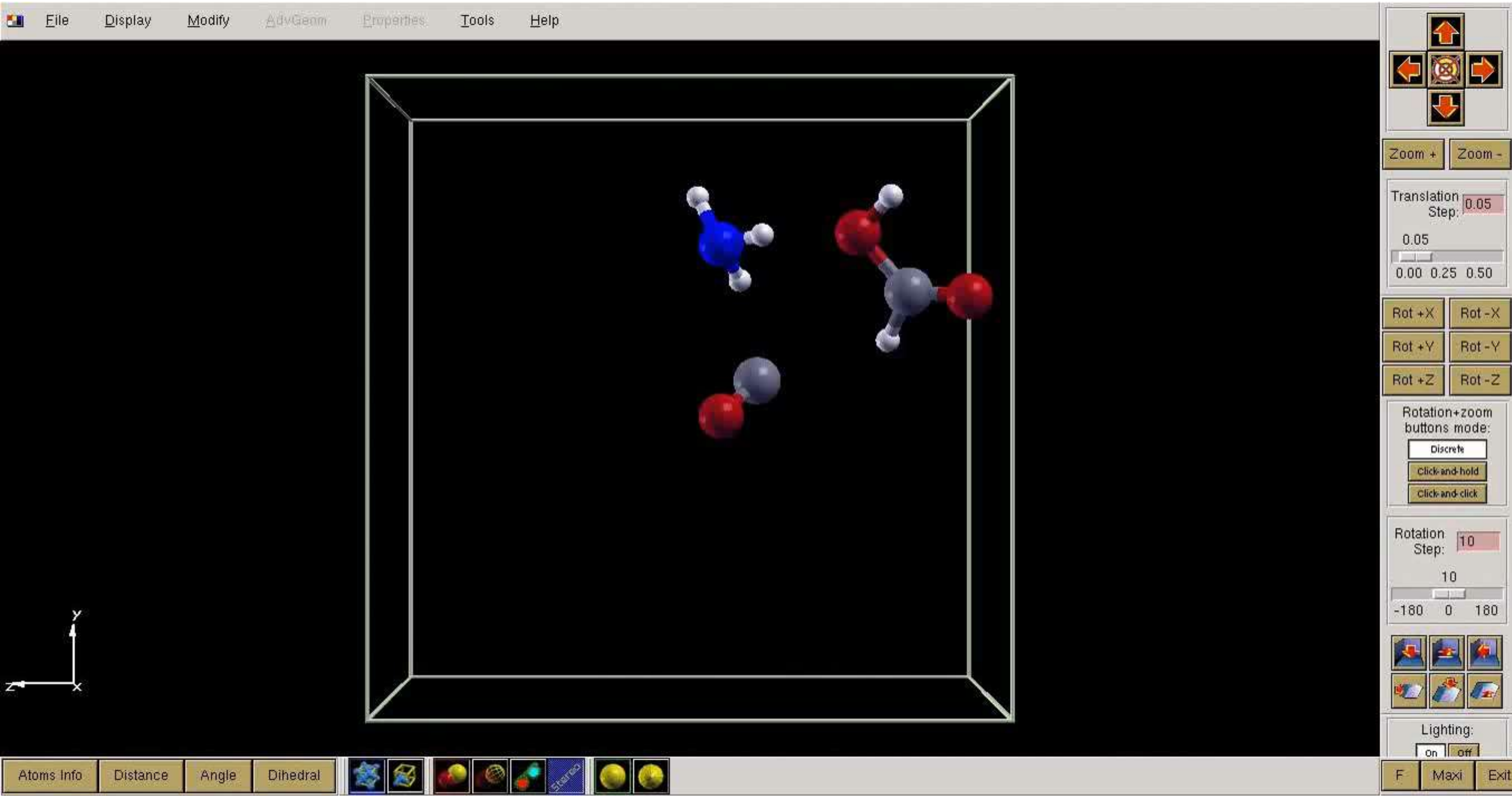
- <u>Spontaneous formation of formic acid and formamide!</u>





AMS and F. Saija, PNAS 111, 13768 (2014)

In silico Miller experiments – II
(Field-induced) Formation of formamide



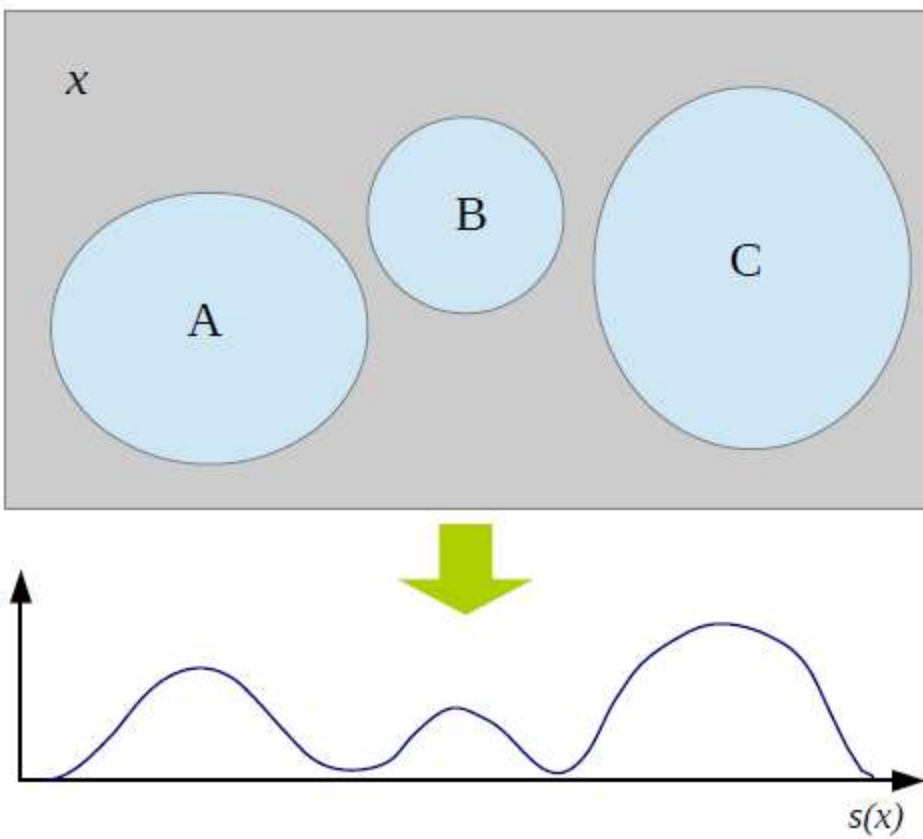
AMS and F. Saija, PNAS 111, 13768 (2014)

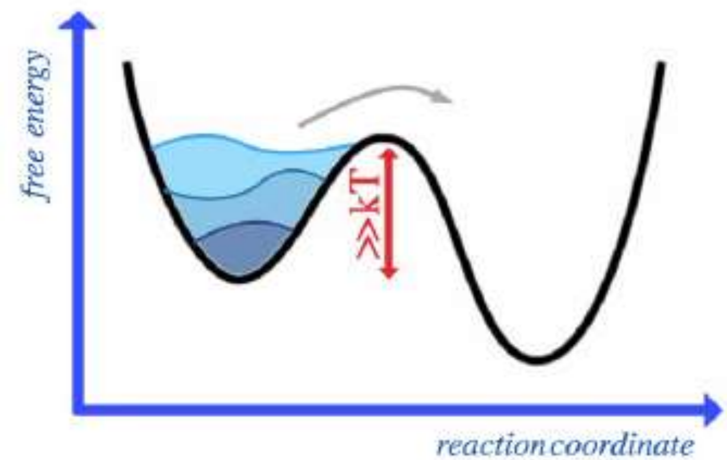
Why are we here?

- Miller's experiment: philosophy, biology, Earth science, chemistry… physics?
- 2014: can we retrace it, step by step, starting from fundamental physics laws?
  - Many-body Schrödinger equation: Density Functional Theory (1963) (W. Kohn, Nobel 1998)
  - Finite temperature: Ab Initio Molecular Dynamics (1985) (R. Car & M. Parrinello)
  - Electric field in quantum mechanics: Berry-phase theory of polarization (1983) (R. Resta, D. Vanderbilt, 1993)
  - Advanced thermodynamics: metadynamics (A. Laio & M. Parrinello 2002)

In silico Miller experiments – II
(Field-induced) Formation of formamide

- ❑ Free-energy landscape ? Metadynamics !



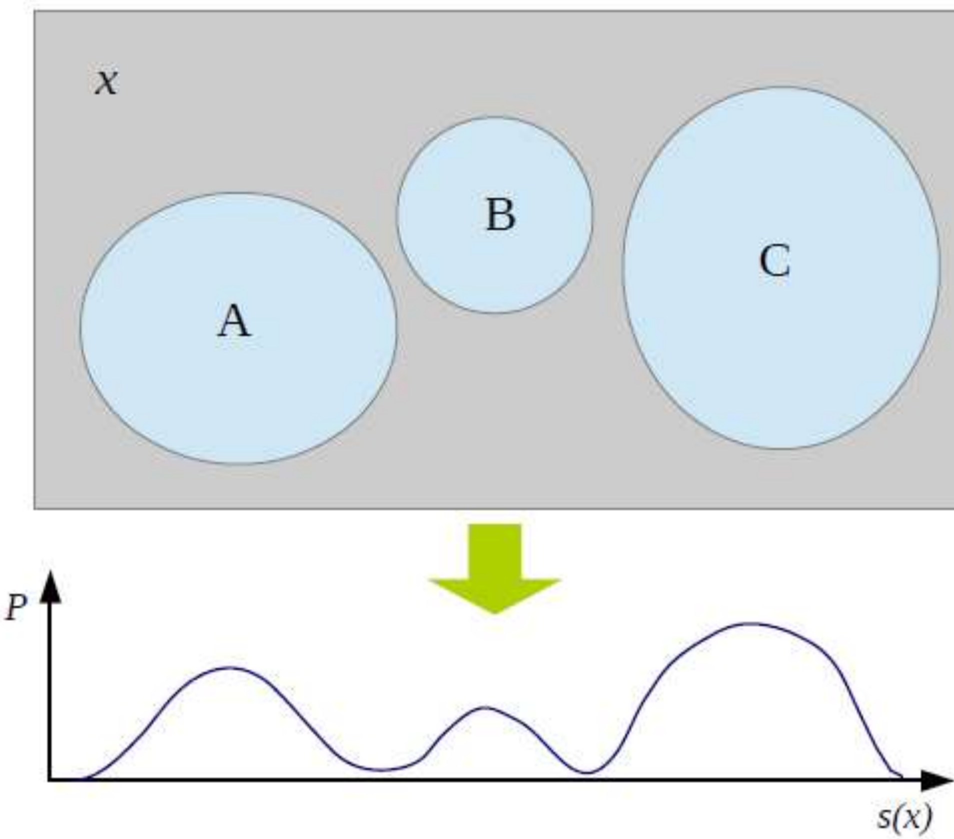


$$P(s) = \lim_{t \to \infty} \frac{1}{t} \int_0^t dt \ \delta(s - s(x(t)))$$

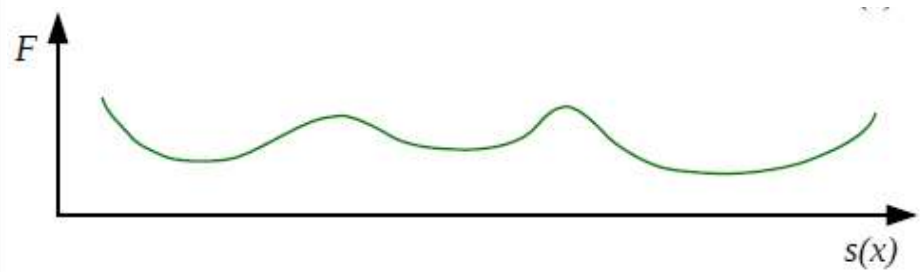
A. Laio & M. Parrinello, PNAS 99, 12562 (2002)

In silico Miller experiments – II
(Field-induced) Formation of formamide

- Free-energy landscape ? Metadynamics !



$$P(s) = \lim_{t \to \infty} \frac{1}{t} \int_0^t dt \; \delta(s - s(x(t)))$$



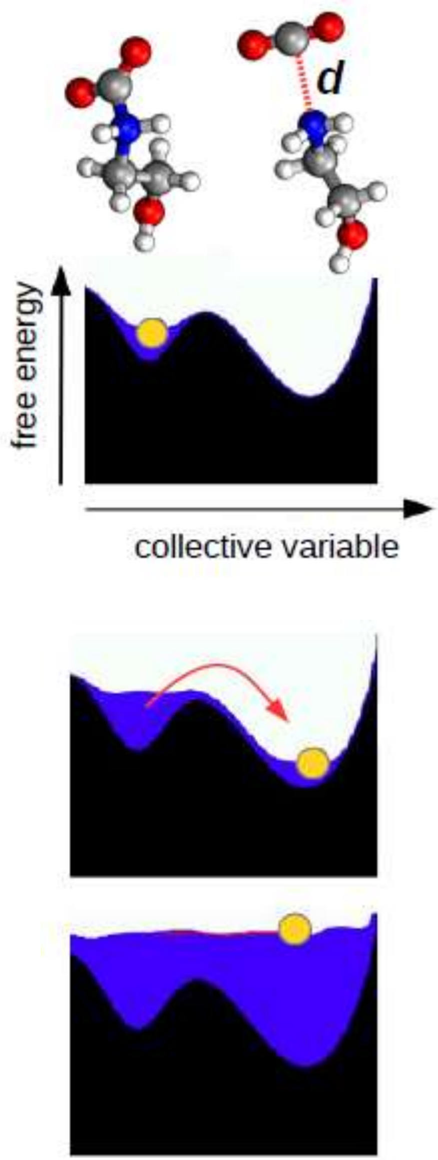
$$F(s) = -\frac{1}{\beta} \log P(s)$$

$$P(s) = \frac{e^{-\beta F(s)}}{\int ds' e^{-\beta F(s')}}$$

$$F(s) = -\frac{1}{\beta} \log \left(\int dx \; e^{-\beta U(x)} \; \delta(s - s(x)) \right)$$

A. Laio & M. Parrinello, PNAS 99, 12562 (2002)

Metadynamics



molecular dynamics

+

hystory-dependent bias potential

$$U^B(s,t) = \sum_{t_1,\ t_2,\ \dots\ <t} \omega \exp\left(-\frac{(s-s(t_i))^2}{2\sigma^2}\right)$$

- accelerated exploration
- reconstruction of the equil. free energy landscape

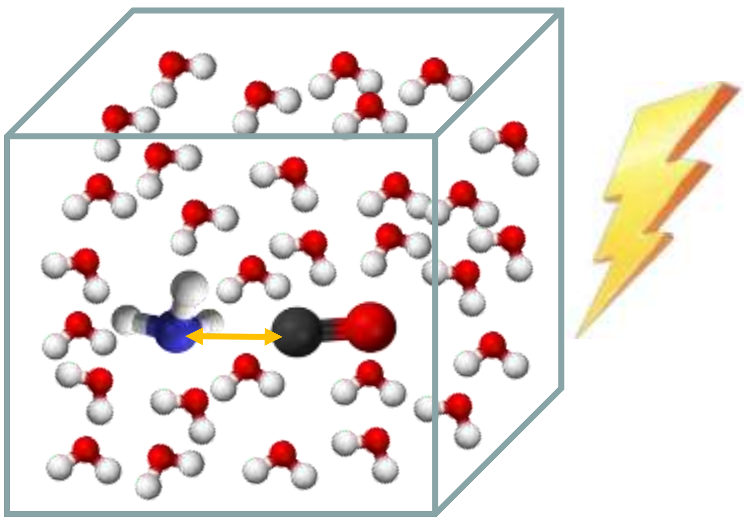
$$\lim_{t\to\infty} U^B(s,t) \approx -F(s)$$

A. Laio & M. Parrinello, PNAS 99, 12562 (2002)

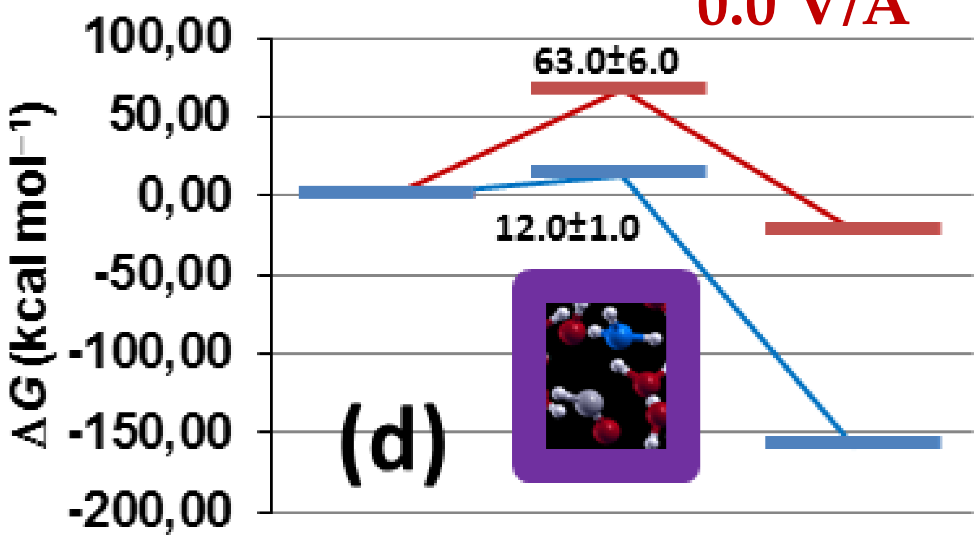
In silico Miller experiments – II
(Field-induced) Formation of formamide

- Free-energy landscape ? Metadynamics !
- Metadynamics study of formamide

$$CO + NH_3 \rightarrow HCONH_2 \rightarrow HCN + H_2O$$



0.0 V/Å

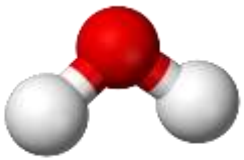


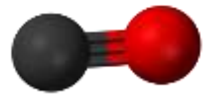
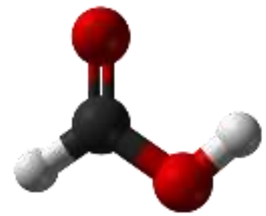
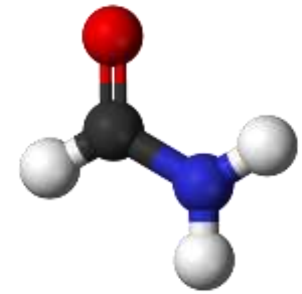
0.5 V/Å

AMS and F. Saija, PNAS 111, 13768 (2014)

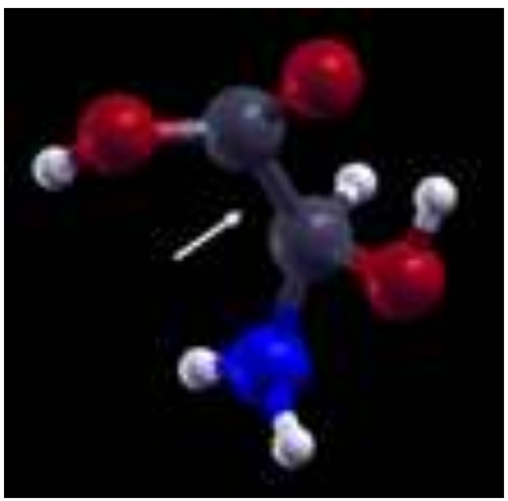
In silico Miller experiments – III
From formamide and formic acid to amino-acids

- Start: new molecules in strong fields



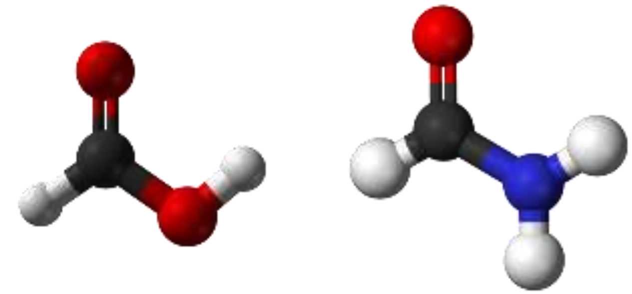
- Formation of hydroxyglycine…



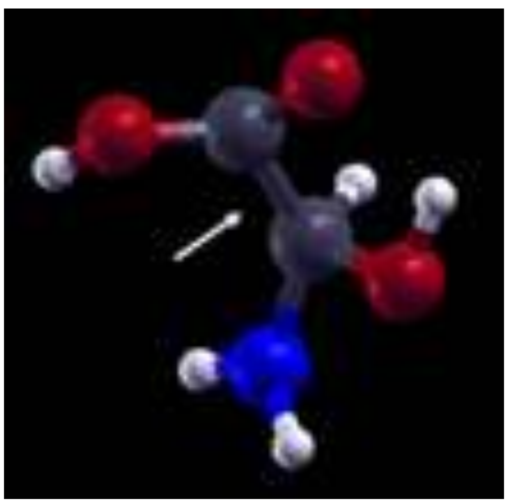
AMS and F. Saija, PNAS 111, 13768 (2014)

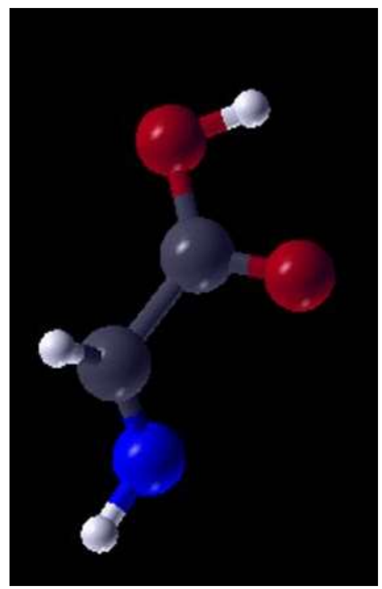
In silico Miller experiments – III
From formamide and formic acid to amino-acids

- ❑ Start: new molecules in strong fields



- ❑ …evolution into dehydroglycine…





AMS and F. Saija, PNAS 111, 13768 (2014)

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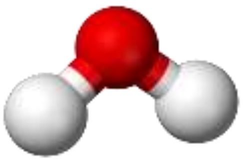
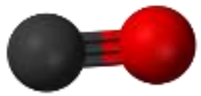
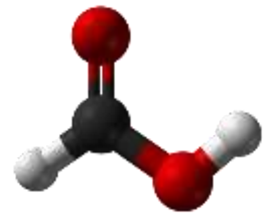
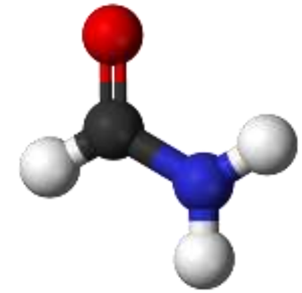
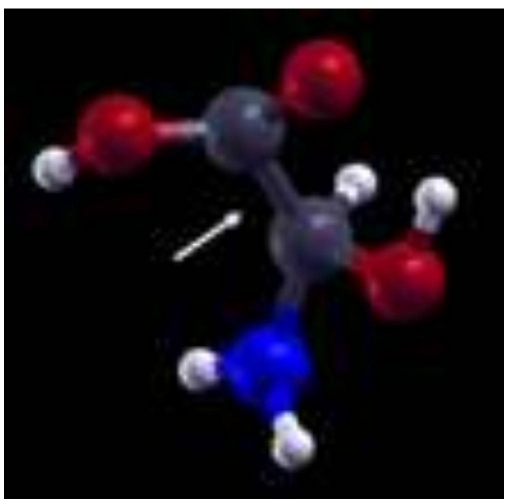
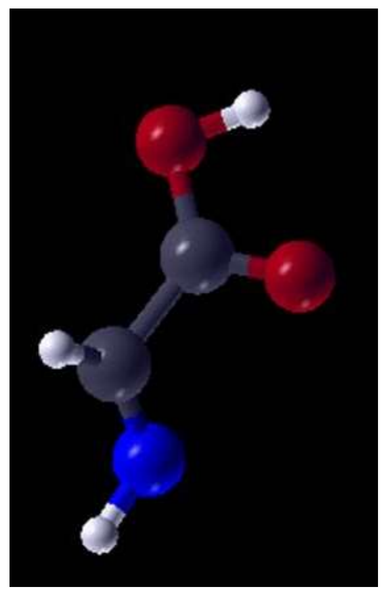
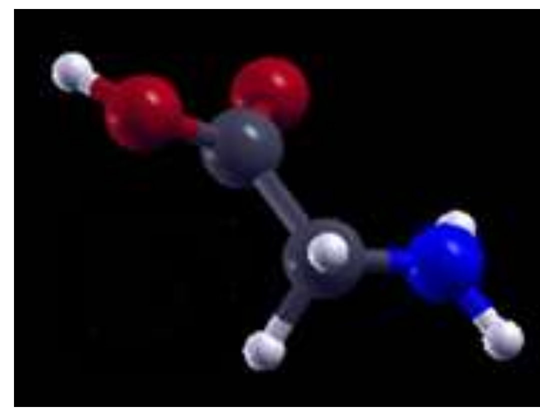


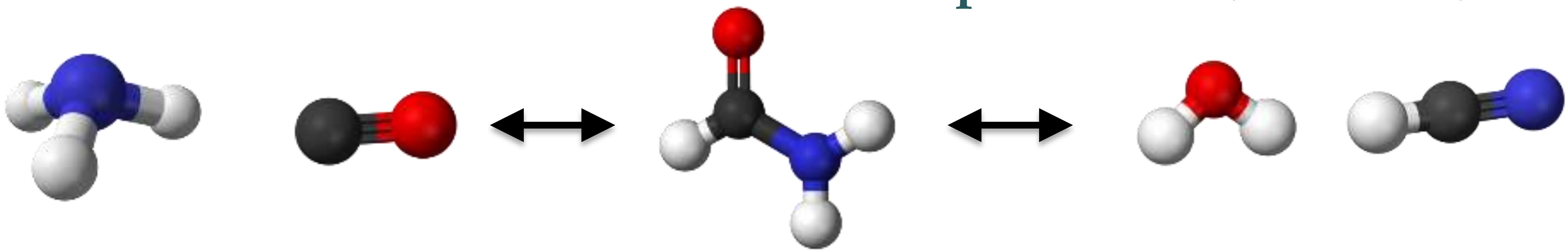
- … and finally glycine !!

AMS and F. Saija, PNAS 111, 13768 (2014)

Prebiotic chemistry & formamide ?

- Formamide not detected in Miller experiments (short life)



- Forms glycine under discharge? A recent study!!

85. Walther Löb: Über das Verhalten des Formamids unter der Wirkung der stillen Entladung. Ein Beitrag zur Frage der Stickstoff-Assimilation.

[Aus der Chemischen Abteilung des Virchow-Krankenhauses zu Berlin.]

(Eingegangen am 10. Febr. 1913; vorgetr. in der Sitzung am 9. Dezbr. 1912.)

$$2H.CO.NH_2 \longrightarrow \begin{array}{l} CO.NH_2 \\ \dot{} \\ CO.NH_2 \end{array} + H_2 \qquad \begin{array}{l} CO.NH_2 \\ \dot{} \\ COOH \end{array} \longrightarrow \begin{array}{l} CH_2.NH_2 \\ \dot{} \\ COOH \end{array}$$

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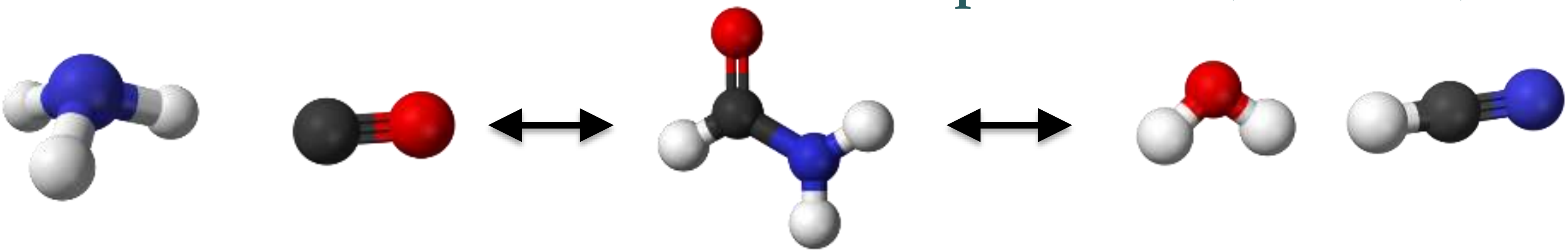


- Suggested as THE key compound in prebiotic chemistry

Available online at www.sciencedirect.com

SciVerse ScienceDirect

Physics of Life Reviews 9 (2012) 84–104

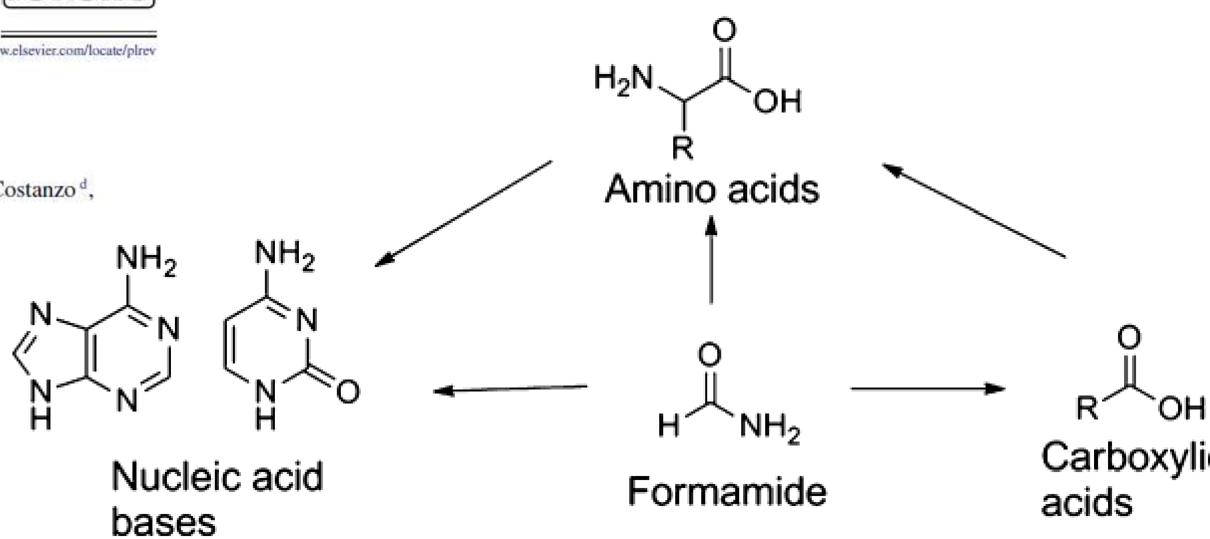
PHYSICS of LIFE reviews

www.elsevier.com/locate/plrev

Review

Formamide and the origin of life

Raffaele Saladino[a], Claudia Crestini[b], Samanta Pino[c], Giovanna Costanzo[d], Ernesto Di Mauro[c,*]



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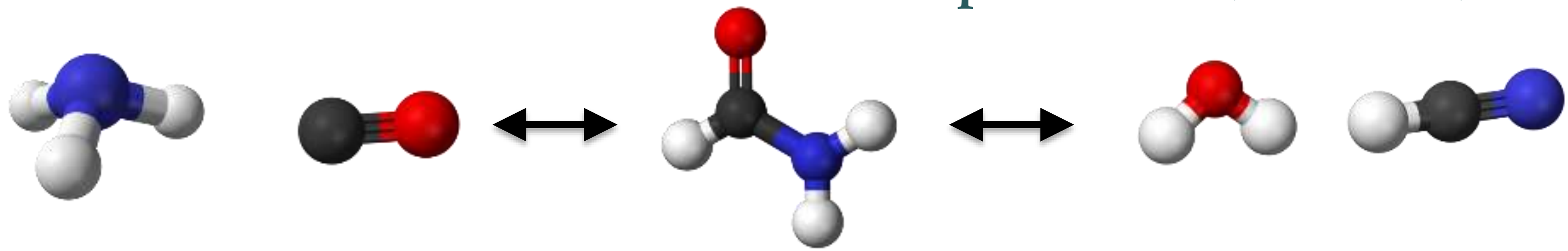


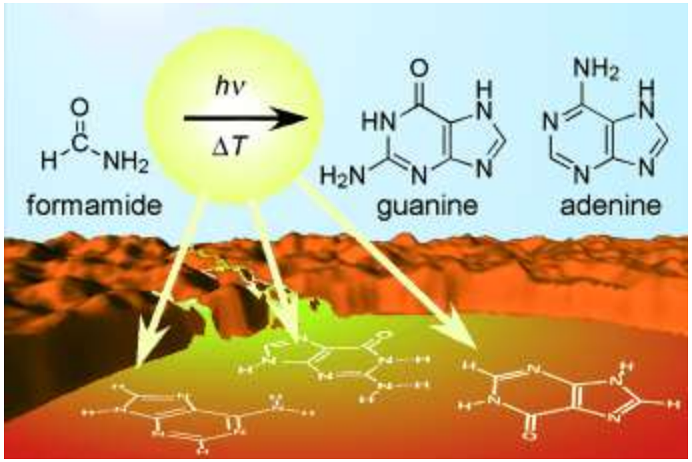
- ❑ Involved in the “missing G” quest

CHEMBIOCHEM

DOI: 10.1002/cbic.201000074

Guanine, Adenine, and Hypoxanthine Production in UV-Irradiated Formamide Solutions: Relaxation of the Requirements for Prebiotic Purine Nucleobase Formation

Hannah L. Barks,[a] Ragan Buckley,[a] Gregory A. Grieves,[a] Ernesto Di Mauro,[b] Nicholas V. Hud,*[a] and Thomas M. Orlando*[a]



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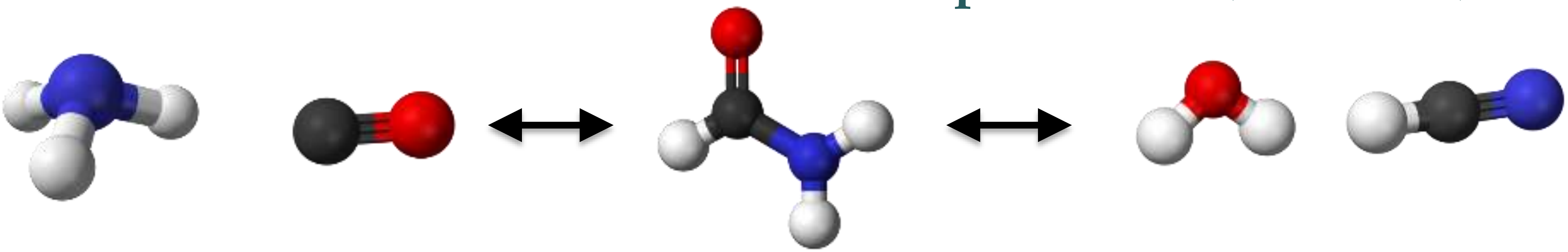
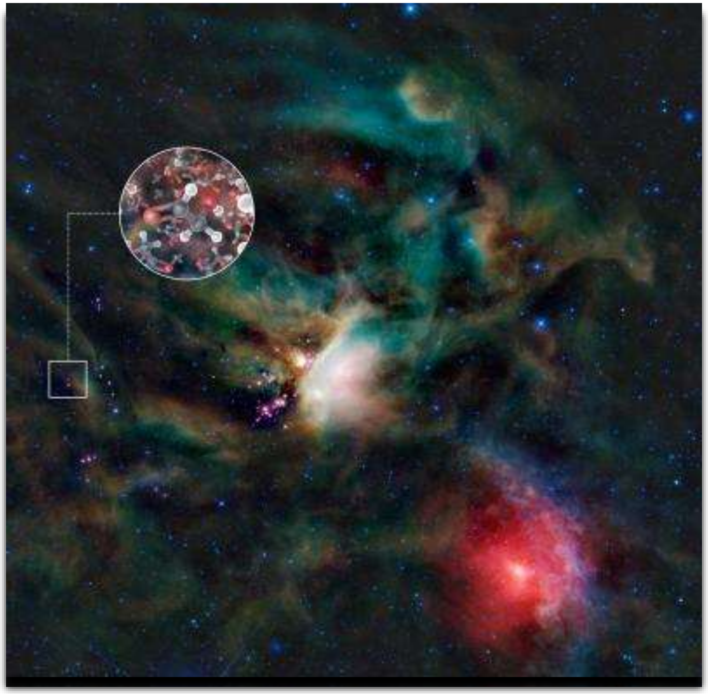


- Abundant in protostars



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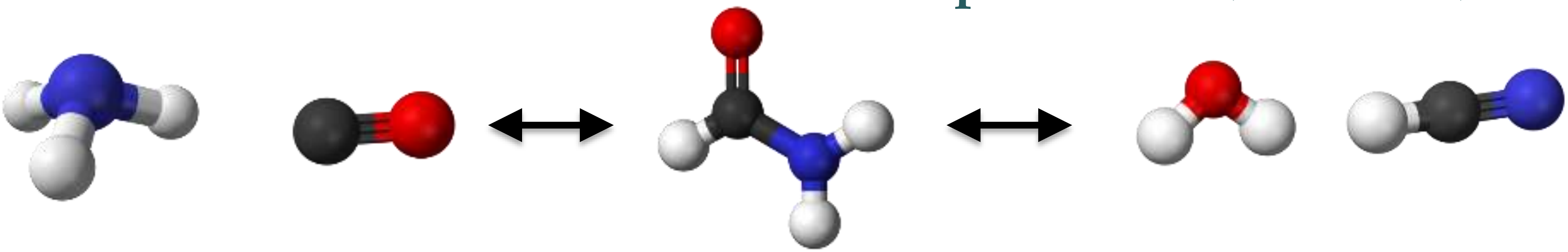

- ❑ Observed in recent ab initio and experimental prebiotic chemistry studies under different, “meteoritic” condition

nature chemistry ARTICLES
PUBLISHED ONLINE: 12 SEPTEMBER 2010 | DOI: 10.1038/NCHEM.827

Synthesis of glycine-containing complexes in impacts of comets on early Earth

Nir Goldman*, Evan J. Reed†, Laurence E. Fried, I.-F. William Kuo and Amitesh Maiti

Delivery of prebiotic compounds to early Earth from an impacting comet is thought to be an unlikely mechanism for the origins of life because of unfavourable chemical conditions on the planet and the high heat from impact. In contrast, we find that impact-induced shock compression of cometary ices followed by expansion to ambient conditions can produce complexes that resemble the amino acid glycine. Our *ab initio* molecular dynamics simulations show that shock waves drive the synthesis of transient C–N bonded oligomers at extreme pressures and temperatures. On post impact quenching to lower pressures, the oligomers break apart to form a metastable glycine-containing complex. We show that impact from cometary ice could possibly yield amino acids by a synthetic route independent of the pre-existing atmospheric conditions and materials on the planet.

nature geoscience ARTICLES
PUBLISHED ONLINE: 15 SEPTEMBER 2013 | DOI: 10.1038/NGEO1930

Shock synthesis of amino acids from impacting cometary and icy planet surface analogues

Zita Martins[1†], Mark C. Price[2*†], Nir Goldman[3], Mark A. Sephton[1] and Mark J. Burchell[2]

Comets are known to harbour simple ices and the organic precursors of the building blocks of proteins—amino acids—that are essential to life. Indeed, glycine, the simplest amino acid, was recently confirmed to be present on comet 81P/Wild-2 from samples returned by NASA's Stardust spacecraft. Impacts of icy bodies (such as comets) onto rocky surfaces, and, equally, impacts of rocky bodies onto icy surfaces (such as the jovian and saturnian satellites), could have been responsible for the manufacture of these complex organic molecules through a process of shock synthesis. Here we present laboratory experiments in which we shocked ice mixtures analogous to those found in a comet with a steel projectile fired at high velocities in a light gas gun to test whether amino acids could be produced. We found that the hypervelocity impact shock of a typical comet ice mixture produced several amino acids after hydrolysis. These include equal amounts of D- and L-alanine, and the non-protein amino acids α-aminoisobutyric acid and isovaline as well as their precursors. Our findings suggest a pathway for the synthetic production of the components of proteins within our Solar System, and thus a potential pathway towards life through icy impacts.

Prebiotic chemistry & formamide!!

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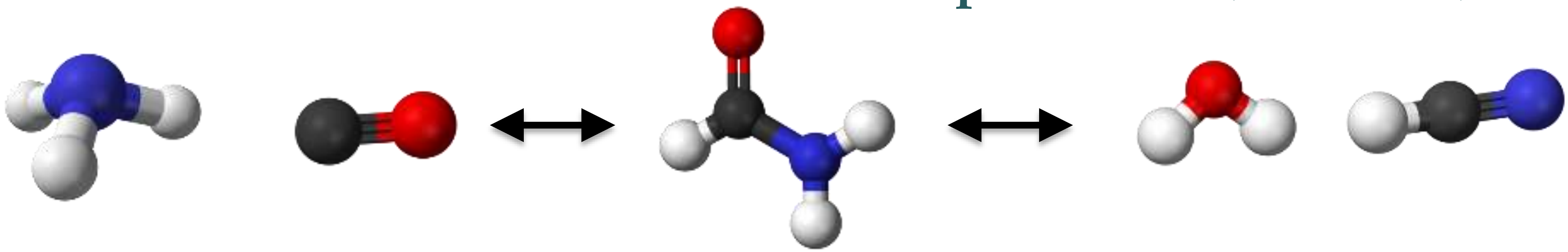


- At the crossroads of prebiotic chemistry (December 2014)

High-energy chemistry of formamide: A unified mechanism of nucleobase formation

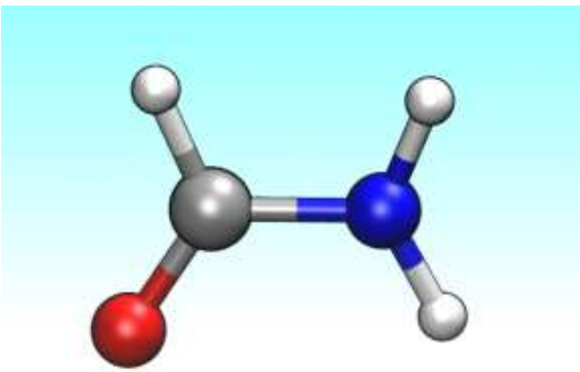
Martin Ferus[a,b], David Nesvorný[c], Jiří Šponer[b,d], Petr Kubelík[a,e], Regina Michalčíková[a], Violetta Shestivská[a], Judit E. Šponer[b,d,1], and Svatopluk Civiš[a,1]

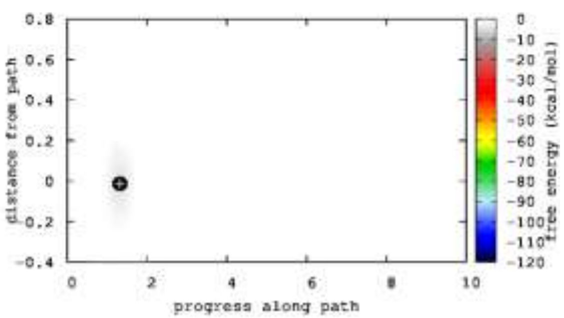
[a]J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, 182 23 Prague 8, Czech Republic; [b]Institute of Biophysics, Academy of Sciences of the Czech Republic, 612 65 Brno, Czech Republic; [c]Department of Space Studies, Southwest Research Institute, Boulder, CO 80302; [d]Central European Institute of Technology, Masaryk University, 625 00 Brno, Czech Republic; and [e]Institute of Physics, Academy of Sciences of the Czech Republic, 182 21 Prague, Czech Republic

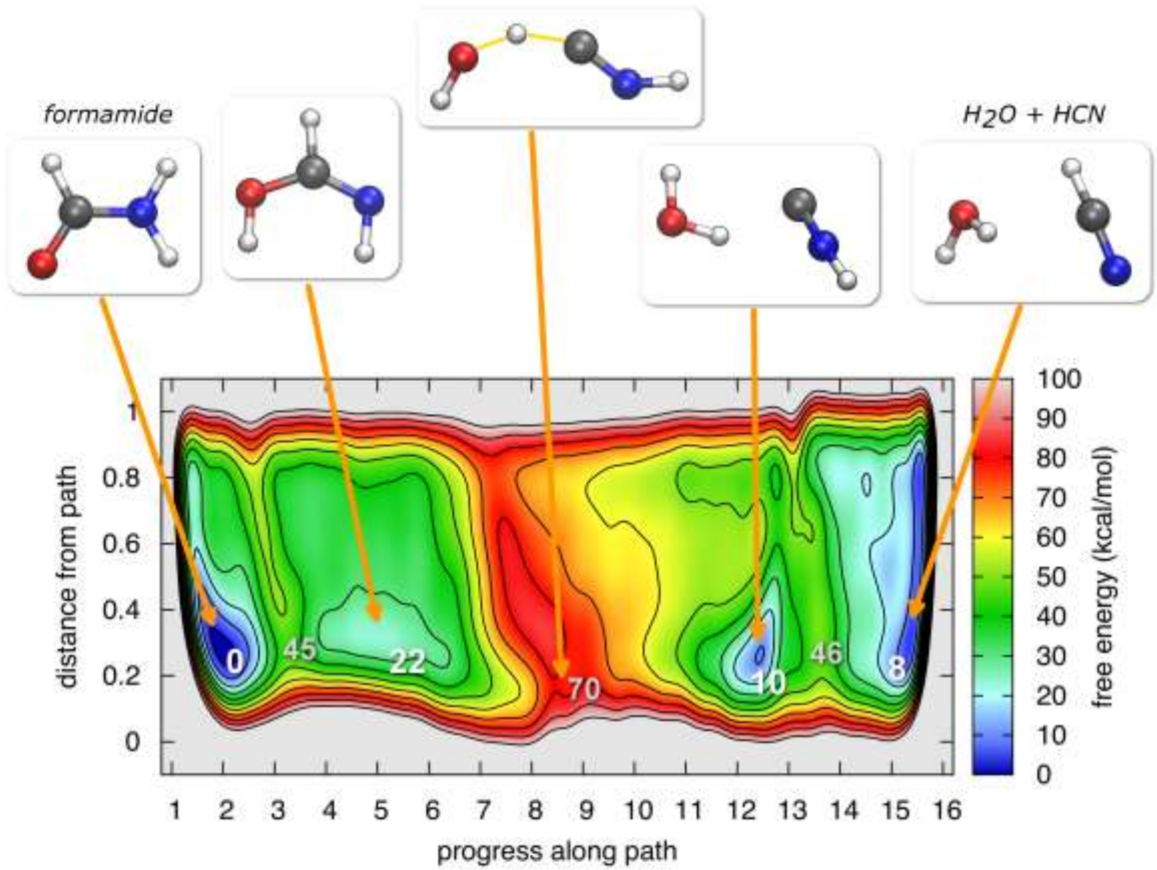
This Feature Article is part of a series identified by the Editorial Board as reporting findings of exceptional significance.

Prebiotic chemistry & formamide!!

❑ **New full-fledged ab initio metadynamics calculations of the formamide breakdown**





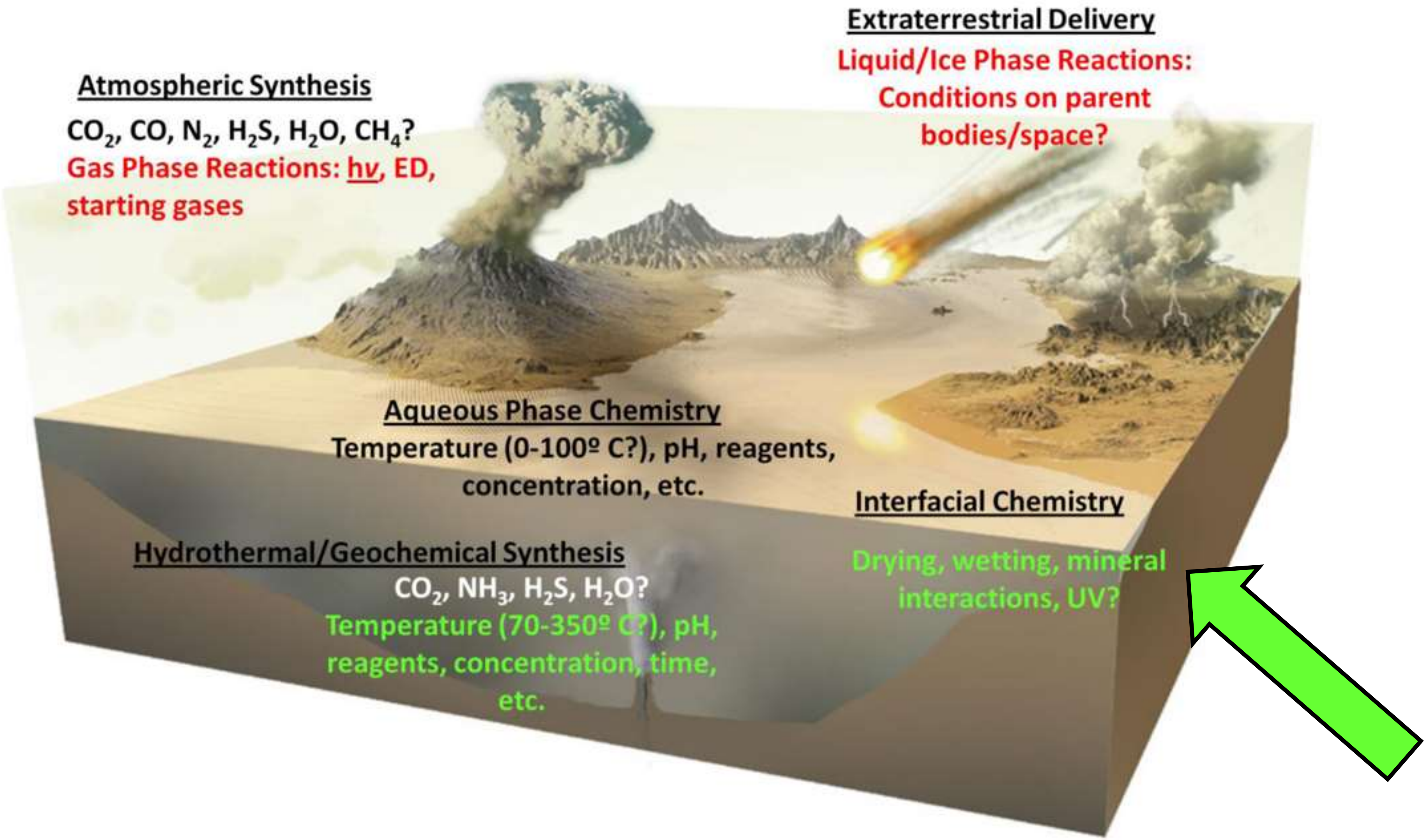


AMS, F. Saija, F. Pietrucci, F. Guyot, PNAS, Jan 2015

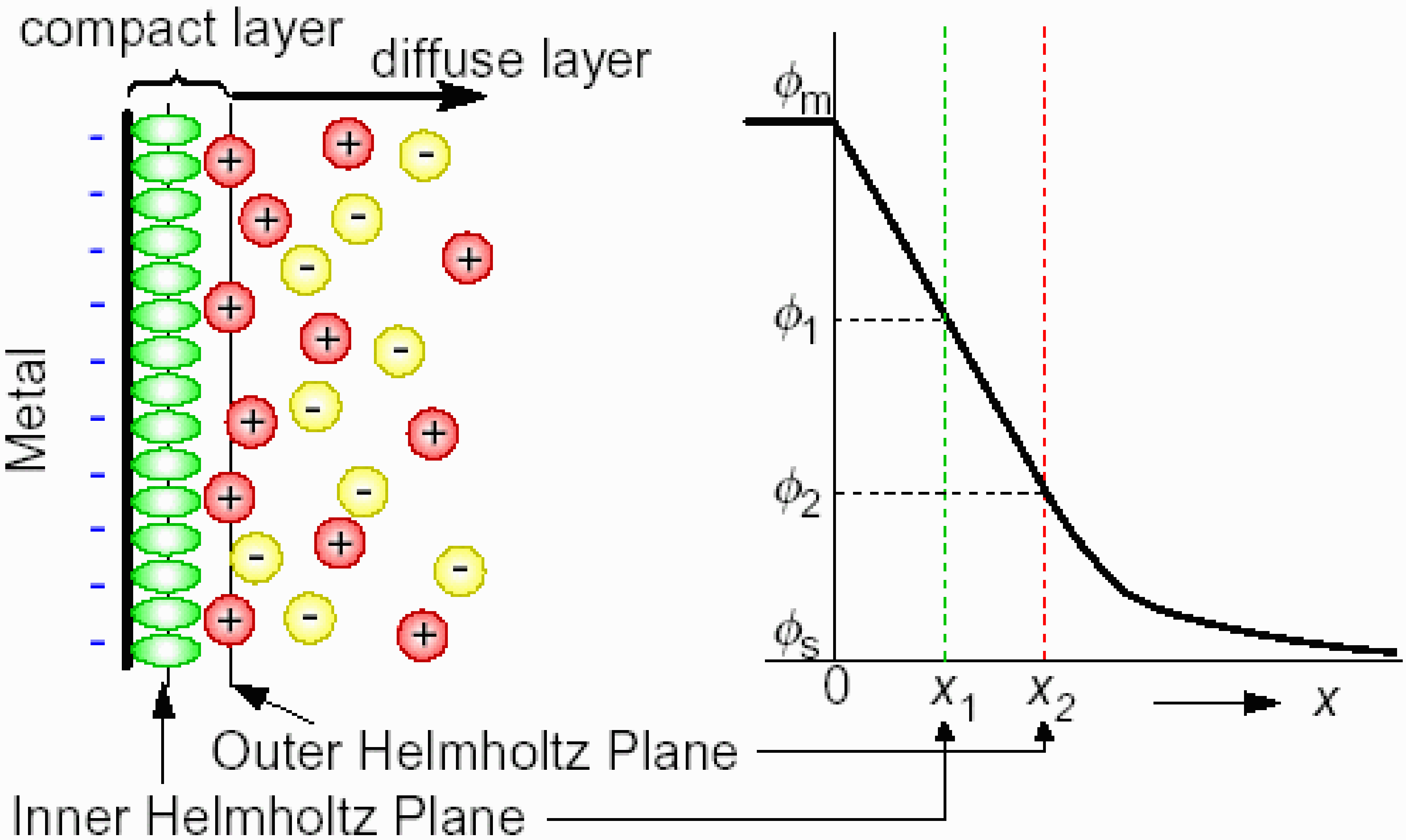
Outline

- Origins of life: from Aristotle to Miller experiments
- The physicist's approach: from complex organisms to electronic wave-functions, and back ?
- *Ab initio* prebiotic chemistry and *in silico* Miller experiments
- Perspectives and conclusions

Mineral surfaces field-induced prebiotic chemistry?

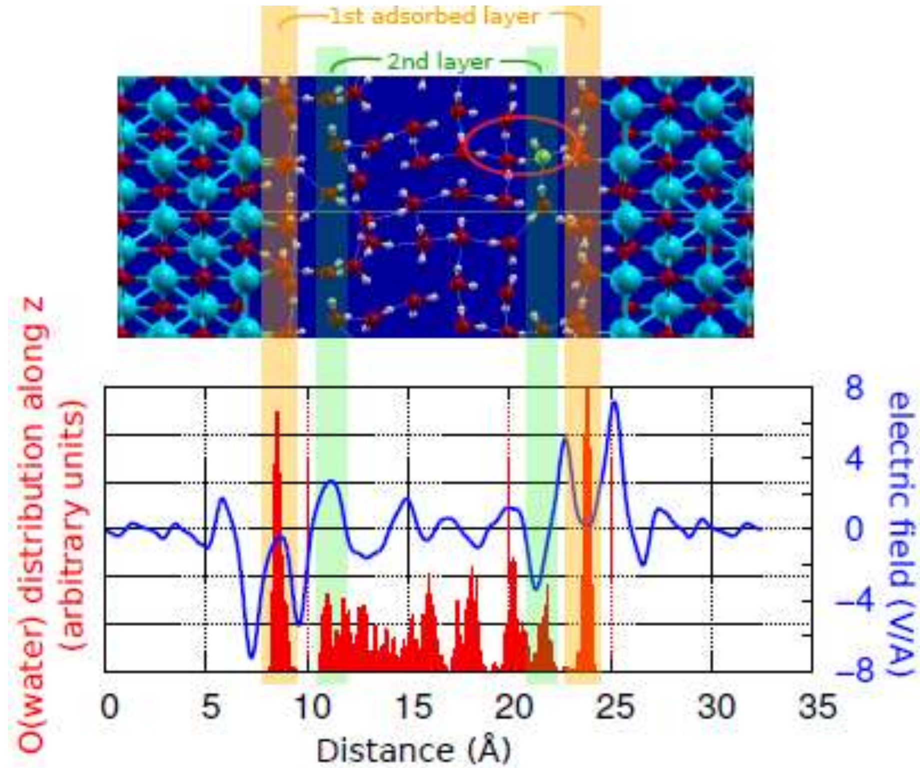


Surface electric field in liquid systems?



Strong electric fields at water/mineral interfaces

❑ Surface field: short-ranged, but around few V/Å



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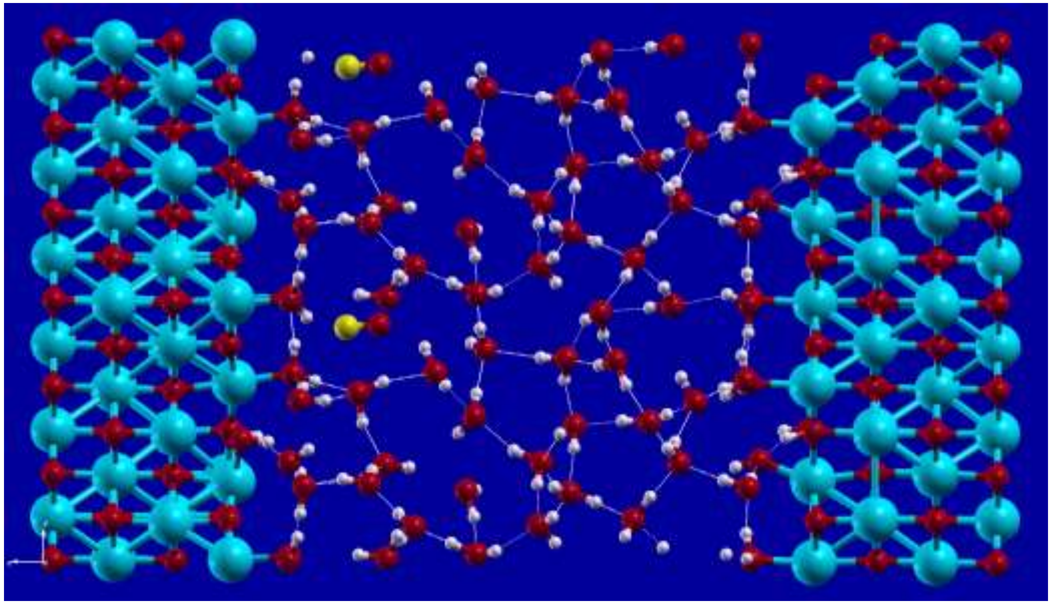

❑ Surface-field-induced “Miller” chemistry and beyond?

In silico Miller experiments, what gives ? Madness !!

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In silico Miller experiments, what gives ? Madness !!

Dr. Stanley Miller (1930–2007), like Frankenstein, stands proudly, arms akimbo, behind his lightning-bolt flask in a piece on Astrobiology Magazine. Yes, he got some glycine and other

Now, to keep the dream alive, Antonino Marco Saitta and colleagues at the Sorbonne in Paris have re-examined Miller's experiment at the quantum level. This, presumably, will breathe new life into the old icon. In computer simulations, they got the glycine all right, and discovered

Sixty-one years now the evolutionists (and NASA, with tax funding), have promoted the Building Blocks of Lie with their Miller icon. We've been crying out like a voice in the wilderness about this phony icon for over a decade (5/02/03). What will it take to get the liars to fess up? They know full well that this experiment has nothing to do with life, but they continue milking it of all the propaganda value they can get to promote atheistic materialism. Debunking the "useful lie" requires some knowledge of organic chemistry

and Orgel falsifying each other. Read Meyer's *Signature in the Cell*. Whatever you do, help stop this scientifically-vacuous, emotionally-poisoned propaganda from doing any more damage to impressionable minds.

Conclusions

- ❑ Ab initio metadynamics & topological variables: a powerful theoretical and computational approach
- ❑ Ab initio Miller experiments and ab initio prebiotic chemistry
- ❑ Formamide identified (again) as a key prebiotic chemistry compound
- ❑ Open question: role of natural surface electric field in chemistry and reactivity
- ❑ Perspectives: Electric-field-induced chemistry of materials ?

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