Division of Life Science : Biological Function and Information Group

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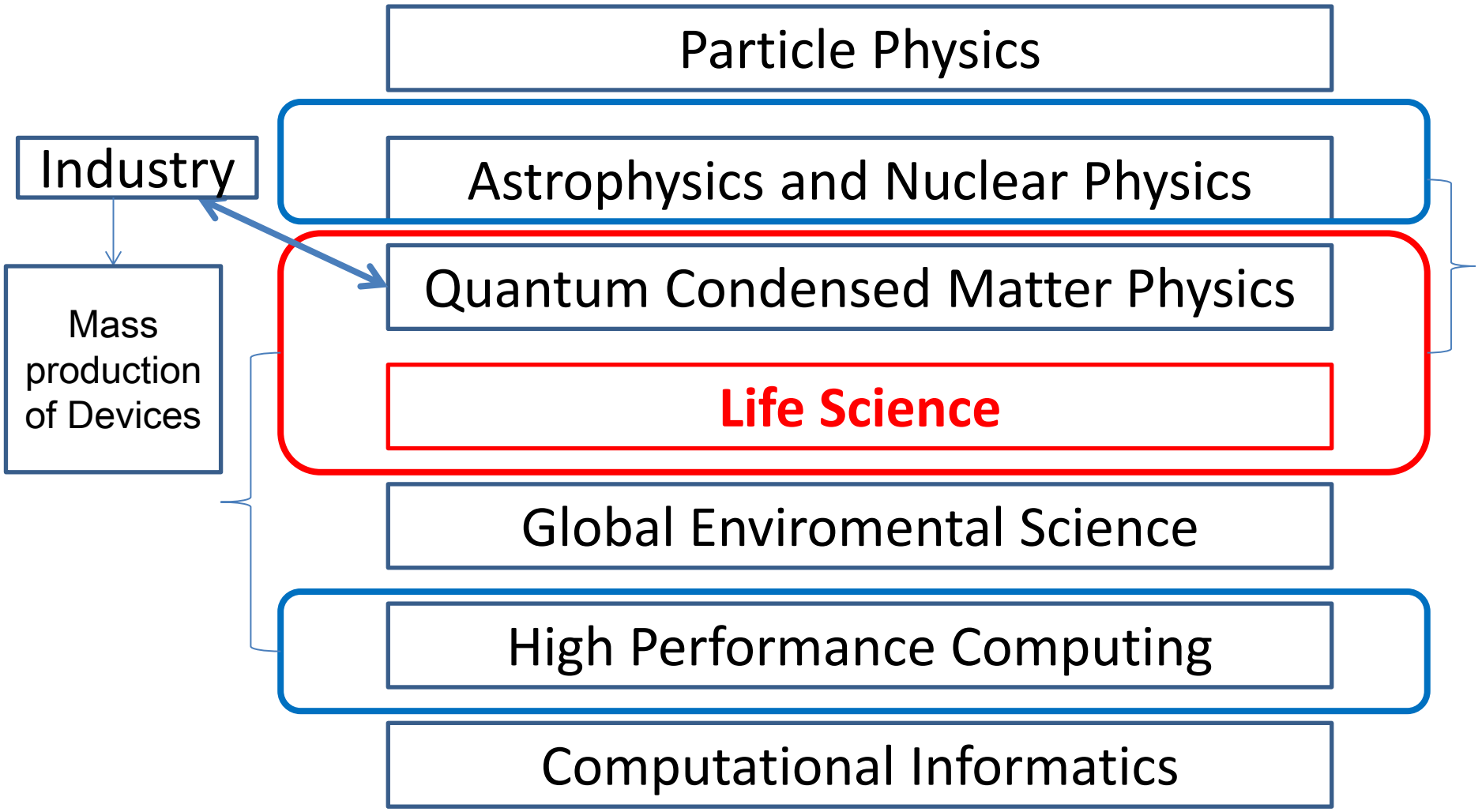
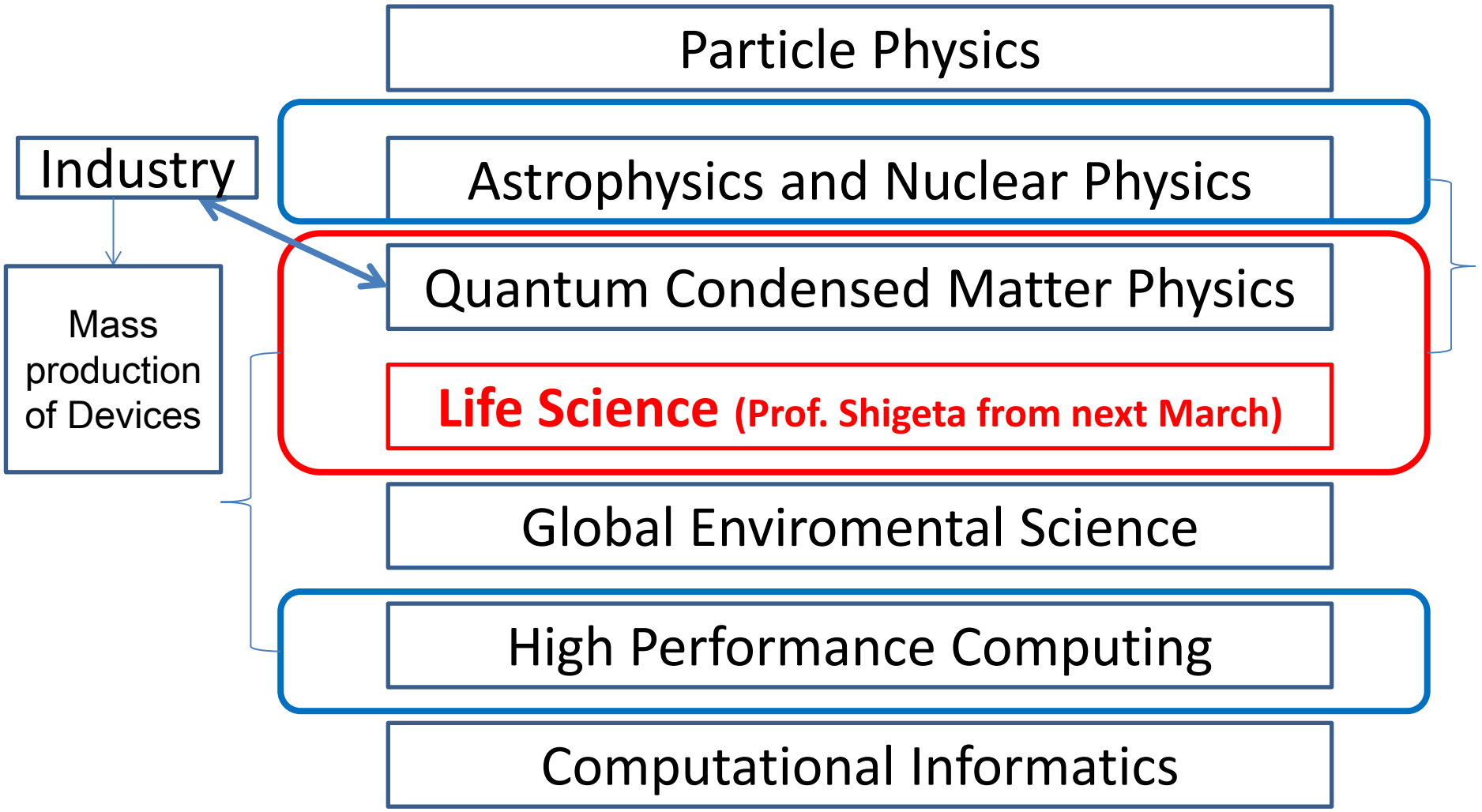
My activity in Center for Computational Sciences (CCS)

- Particle Physics
- Astrophysics and Nuclear Physics
- Quantum Condensed Matter Physics
- Life Science
- Global Enviromental Science
- High Performance Computing
- Computational Informatics

My activity in Center for Computational Sciences (CCS)



My activity in Center for Computational Sciences (CCS)



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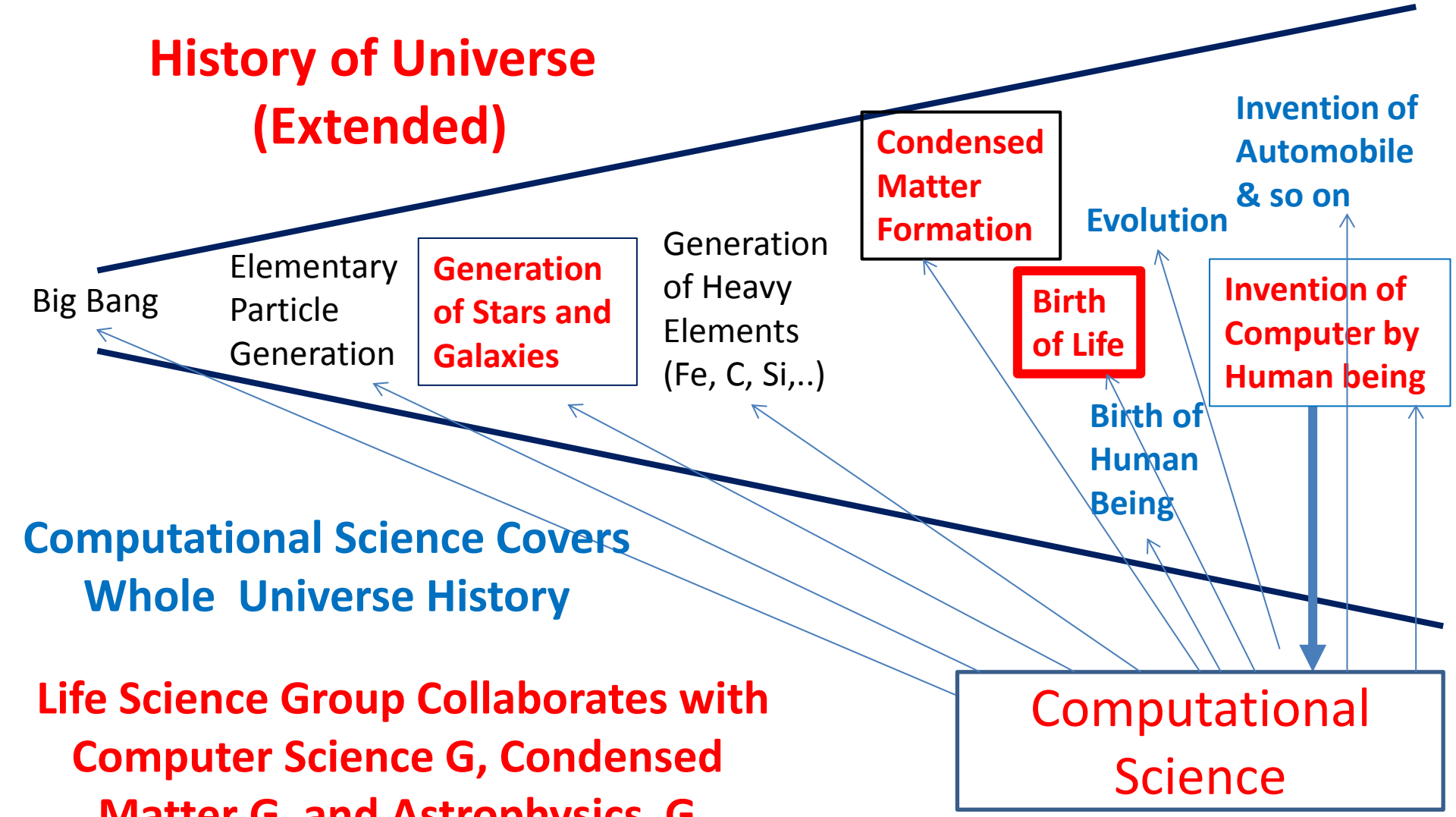
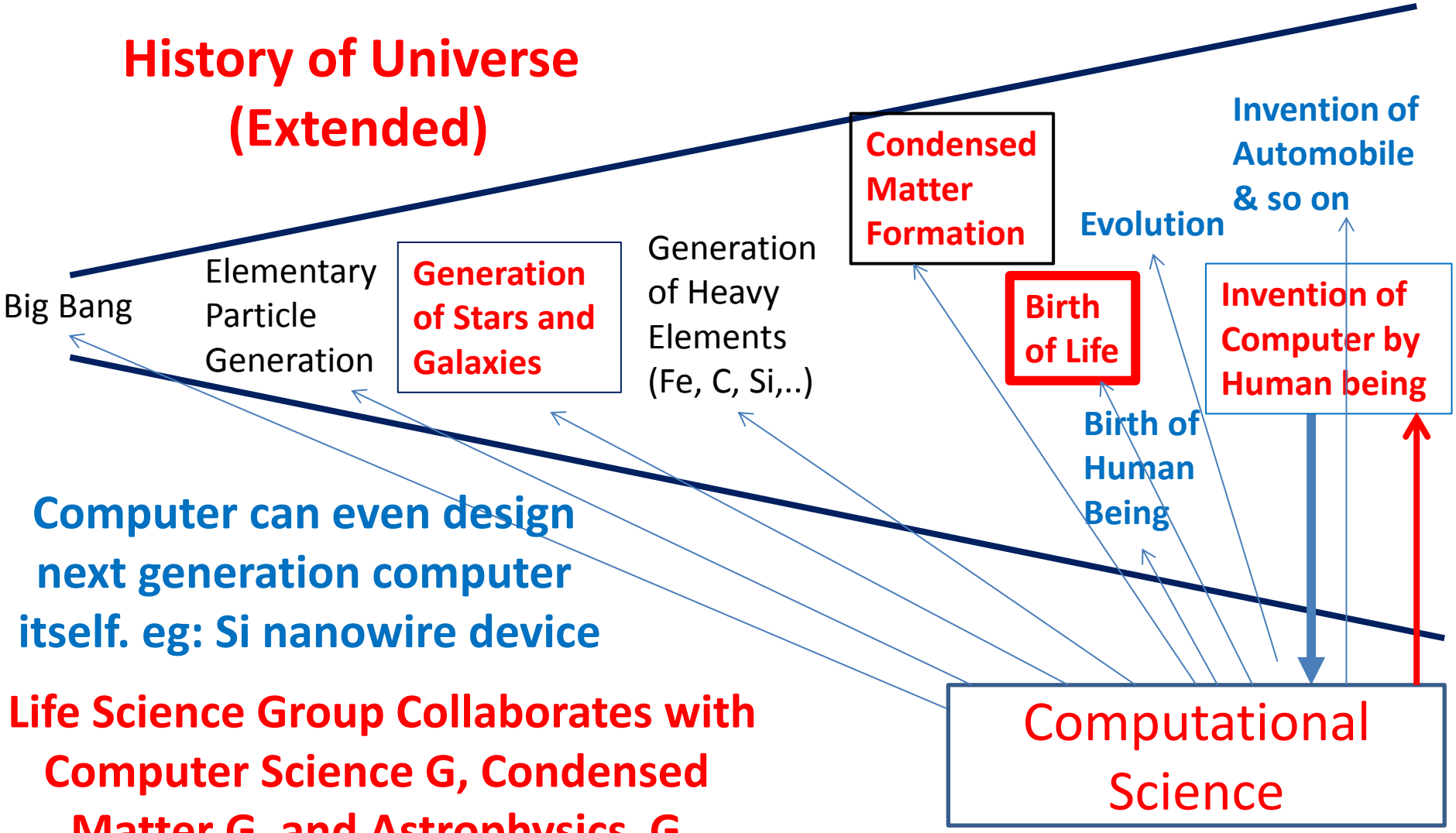
1. Overview of life science group

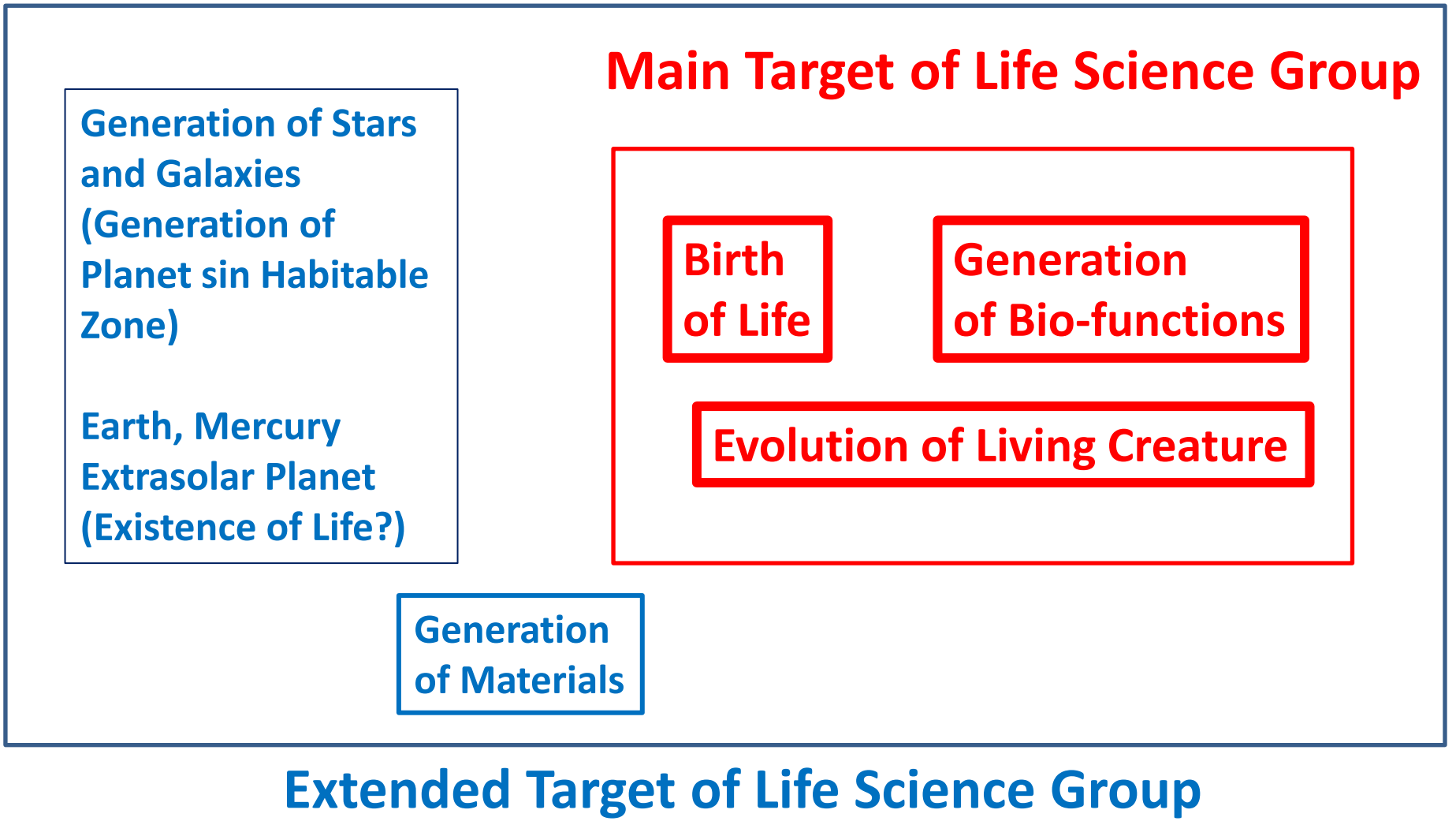


1. Overview of life science group



Overview in more details

Life Science Group Wants to Cover History of Universe Related to Life Science with Other Groups



2.Interaction with Other Fields

- Computer Science Group

  New Computation Algorism

  (GPU, super parallel computers and so on)
- Condensed Matter Group

  First principles (Ab initio) calculation method which

  can predict material properties as well as bio-functions
- Astrophysics Group

  Origin of Life

  - Origin of Excess of L-Amino Acid in living creature
  - Mechanism of habitable planet generation

We believe that astrophysics is very important for life science. (collaborating with Australian University, CNRS (France) as well as Nagoya University and Osaka University and so on)

3. Research Results Summary

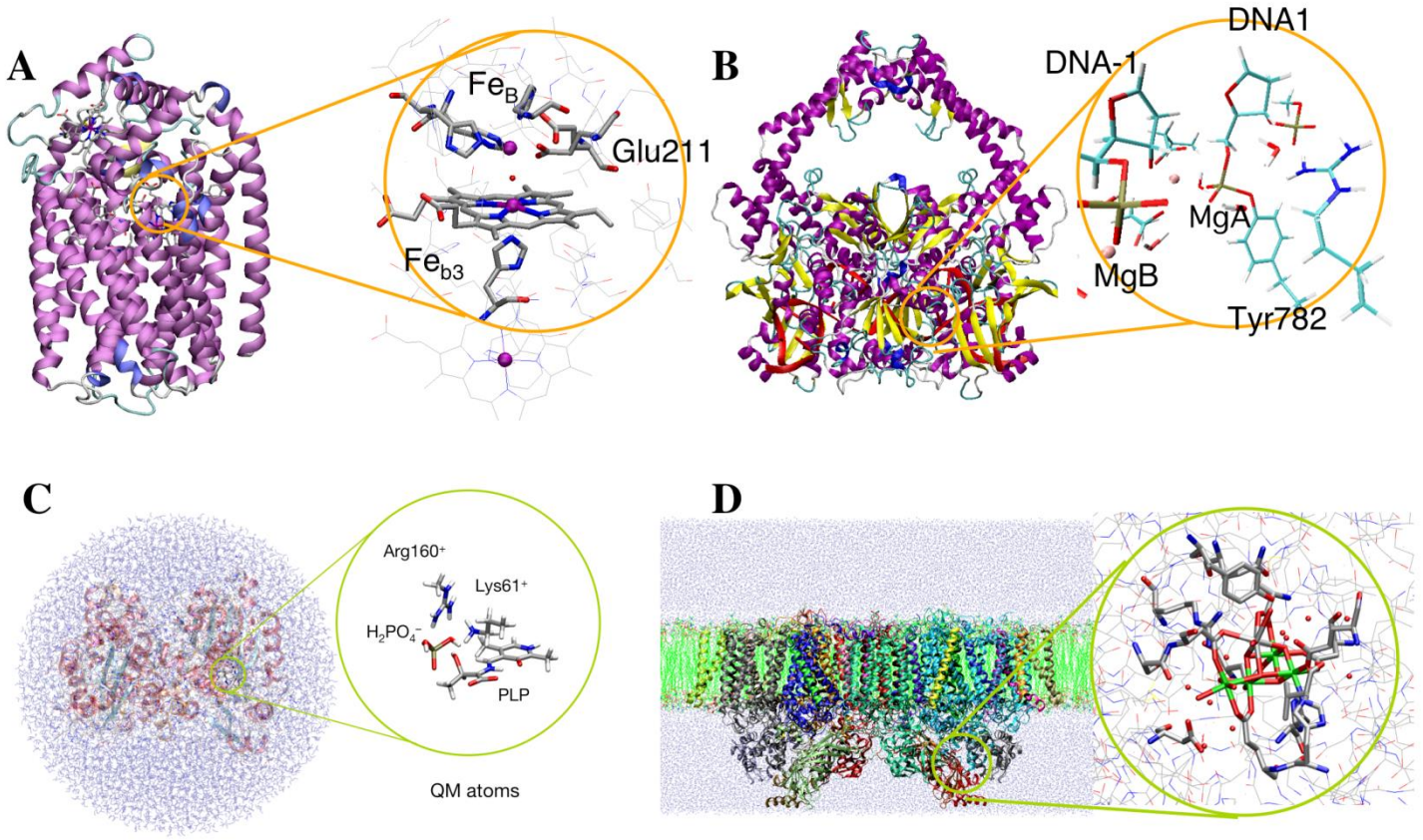
1. Microscopic Origin of Bio-functions
   1.1 Nitric Oxide Reductase
2. Origin of Life (Collaboration with Condensed Matter G and Astrophysics G)
   2.1 Homochirality of Amino Acids in Proteins
   2.2 Approaches towards Generation Mechanism of Habitable Planets

1. Method for Bio-function Research

- QM/MM Approaches is used for describing bio-functional proteins.
- QM regions are calculated by Ab initio quantum chemical approaches
- MM regions are treated by AMBER force fields

1.1 Nitric Oxide Reductase(NOR) (by M. Shoji)

NOR reduces NO to N_2O



Systems used for QM/MM calculations. QM regions are enlarged. (A) NOR, (B) topo, (C) TS, and (D) OEC-PSII.

2. Origin of Life

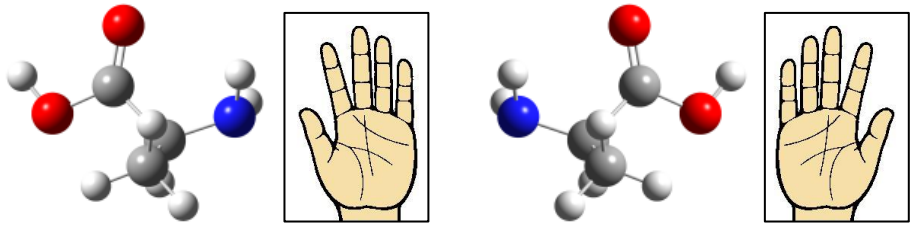
2.1 Homochirality of Amino Acids in Proteins

What is Homochirality?

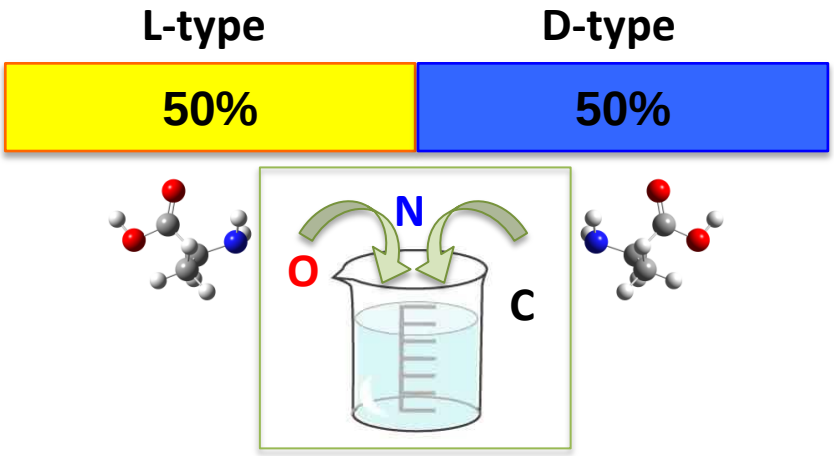
Enantiomer (Miror image isomer)

Amino Acids have two types of enantisomer.

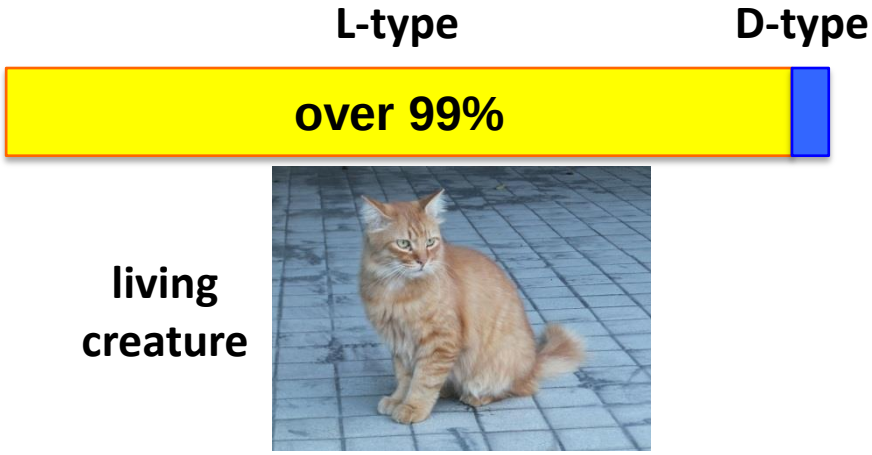
L-type (Left) **D-type (Right)**



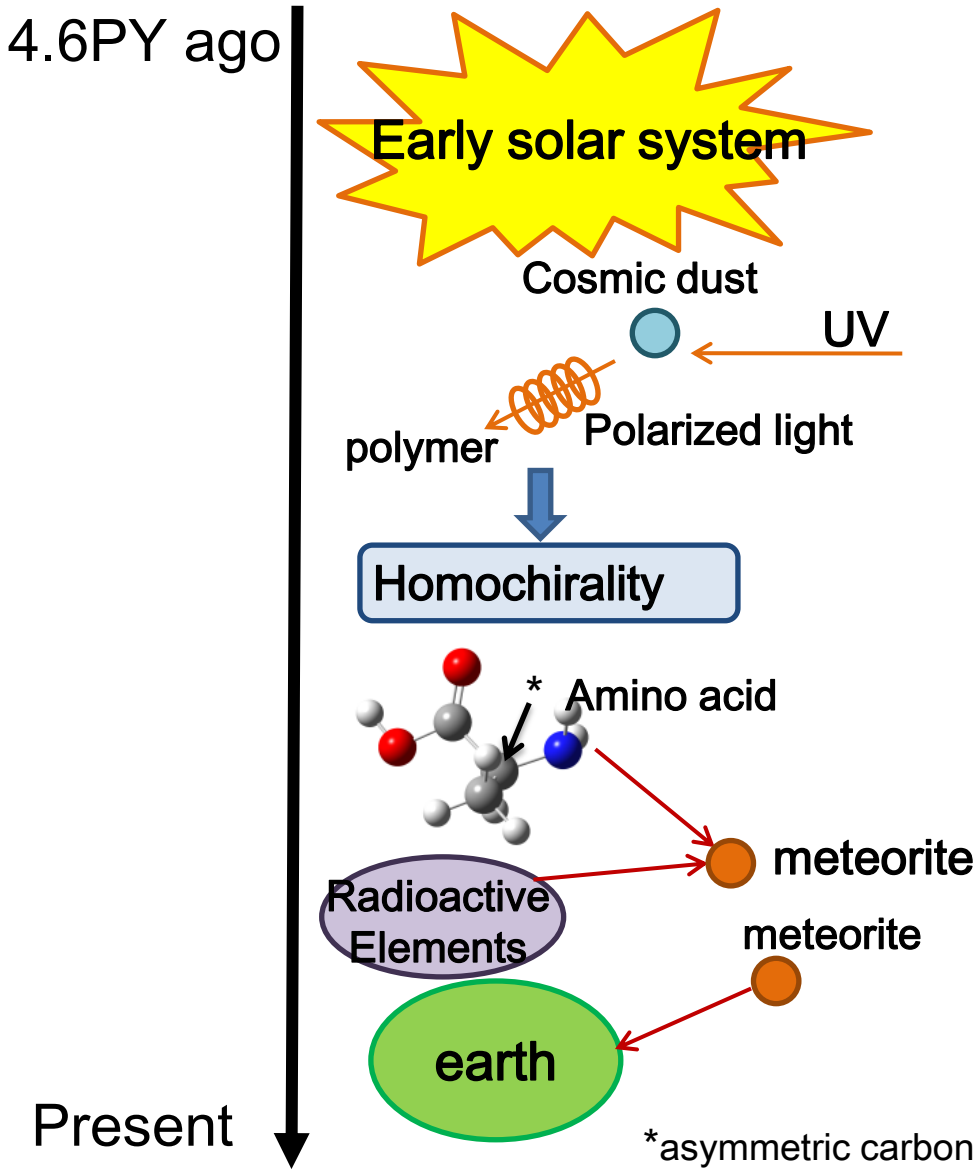
In Chemial Experiments



In living creature



Story of homochirality generation in the early solar system



① Birth of early solar system
→ supernova explosion
→ Present solar system

② Polarized light is generated by the scattering by cosmic dusts

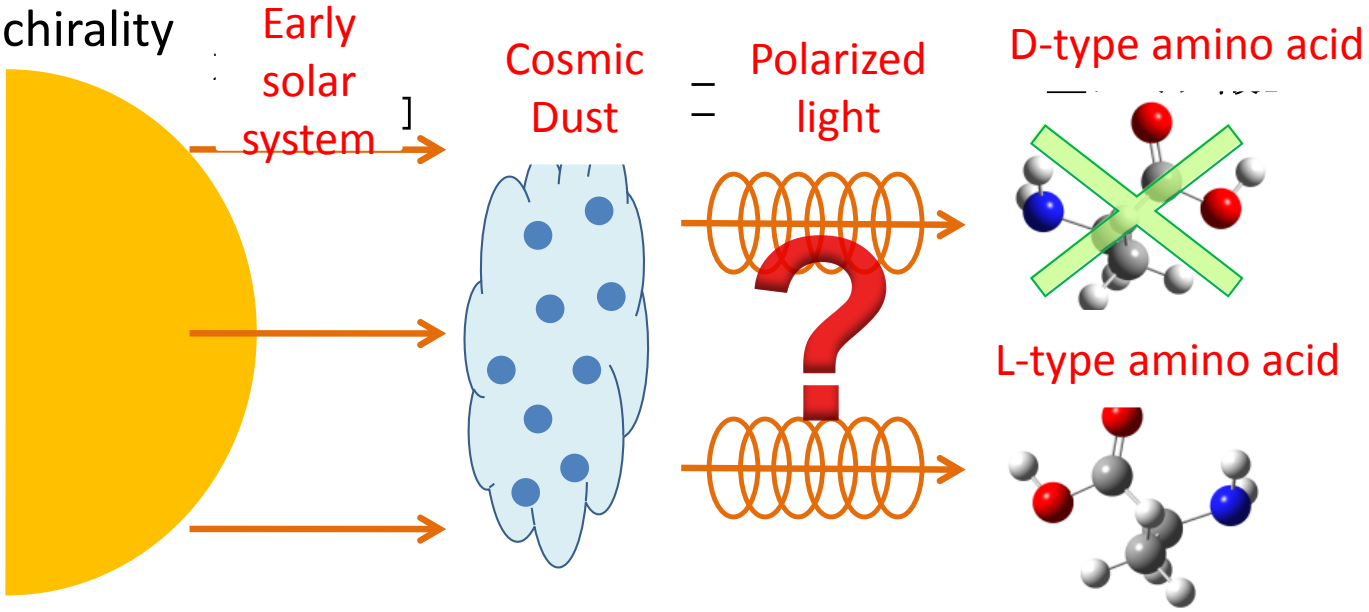
③ Homochiralitiy is generated by the circular polarized light emitssion

④ Meteorite with excess L-type amino acids

⑤ Above meteorites become the origin of life on earth

Purpose of this work

To clarify the mechanism of selective destruction of amino acids.
What kind of light can destruct amino acid selectively to generate homochirality



Chemical experiments cannot clarify the detail mechanism of homochirality.

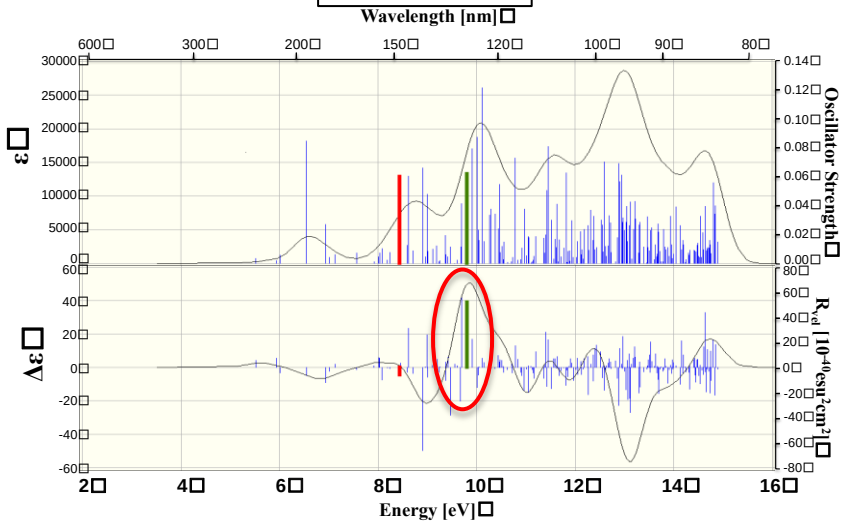
Computational science approach is powerful

Circular dichroism (CD) is calculated by ab initio calculations

CD describes the selective destruction of enantiomer by polarized light

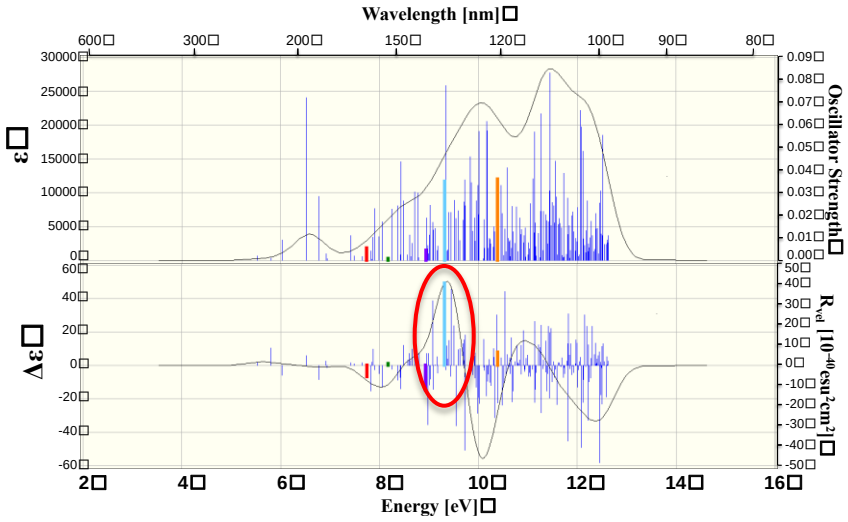
Calculated circular dichroism of alanine and isovaline

Alanine



Curve 2.	126.3524 nm

Isovaline



Curve 4.	133.0155 nm

	Wave length
Alanine	**126.4 nm**
Valine	**113.7 nm** **124.0 nm**
Isovaline	**133.0 nm**

110nm – 135nm
Vacuum ultraviolet region

Conclusion

Homochirality can be generated by the emission of circular polarized light emission in the early solar system

Vacuum ultra violet circular polarized light can generate homochirality of amino acid in living creature （**110-135 nm**）

Cosmic Filter??

2.2 Approaches towards Generation Mechanism of Habitable Planets (A Preliminary Result)

Story of planet generation

There is a missing link for understanding planet formation from cosmic dusts (living place of living creatures).

Collaboration between Astrophysics, Condensed Matter Physics and Life Science is inevitable to overcome this missing link.

- Cosmic dusts get together and formation of planetesimal (very small planet) occurs
- Comic dusts essentially obey fluid mechanics. (Physics of continuum can be applied)
- However, cosmic dusts occasionally behave as inertial particles, and collision of these cosmic dusts is the origin of generation of planetesimal.

Method of numerical simulation of Nervier-Stokes equation

- Incompressible fluid (Future, compressible fluid treatment)
- No magnetic field (Future, magnetic hydromechanics (MHD) treatment)
- Mesh: $256 \times 256 \times 256$
- Time evolution: Runge-Kutta 4^{th} order
- Number of Inertial Particles $16 \times 16 \times 16$

Equation for inertial particle

$$\begin{cases} \dfrac{d\boldsymbol{X}}{dt} = \boldsymbol{V} \\ M\dfrac{d\boldsymbol{V}}{dt} = \boldsymbol{F} \end{cases}$$

$$\boldsymbol{F} = \mu a\left(\boldsymbol{u}-\boldsymbol{V}\right)+\left(\rho_p-\rho_f\right)a^3\boldsymbol{g}$$

$$\begin{cases} \dfrac{d\boldsymbol{X}}{dt} = \boldsymbol{V} \\ \dfrac{d\boldsymbol{V}}{dt} = \dfrac{1}{St}\left(\boldsymbol{u}-\boldsymbol{V}+\boldsymbol{V_T}\right) \end{cases}$$

Stokes Number $St = \dfrac{\beta a^2 U}{\nu L}$

$$\boldsymbol{V_T} = \frac{\left(\beta-1\right)a^2}{\nu U}\boldsymbol{g}$$

※Neglecting gravity

$$\boldsymbol{V_T} = \boldsymbol{0}$$

3. Future plan (by Prof. Shigeta)