Homochirality and information content of the building blocks of life via theoretical spectroscopy

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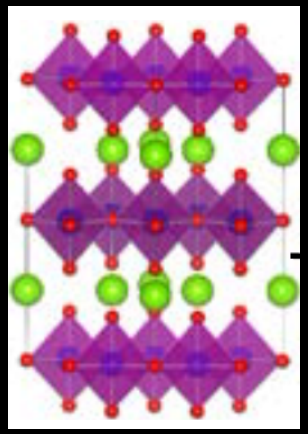
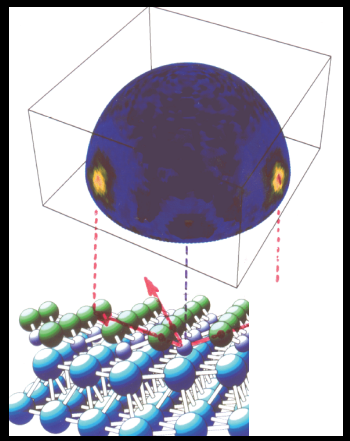
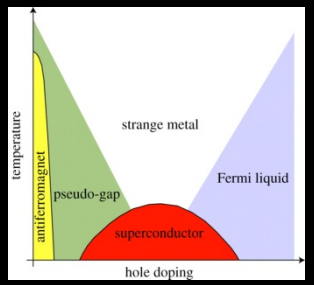
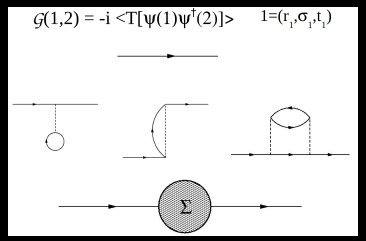
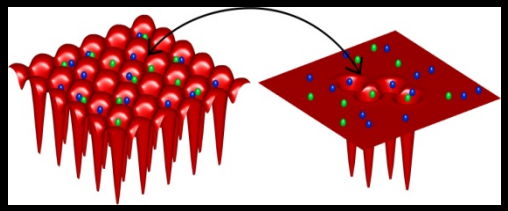


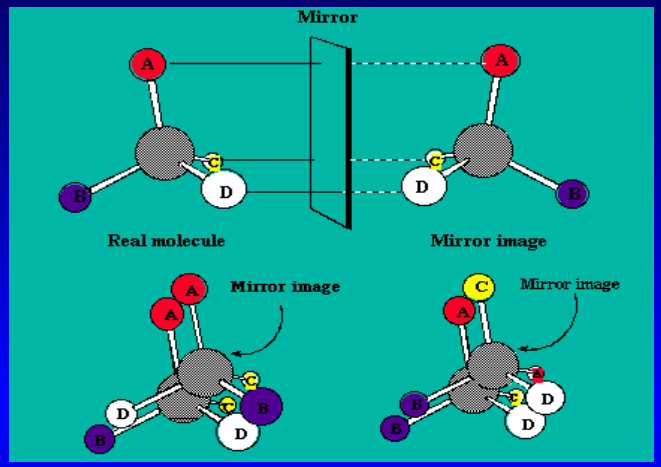


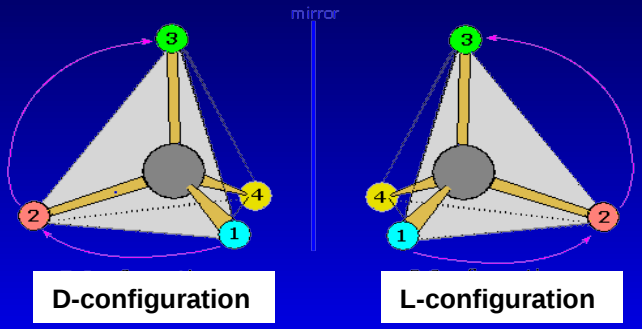


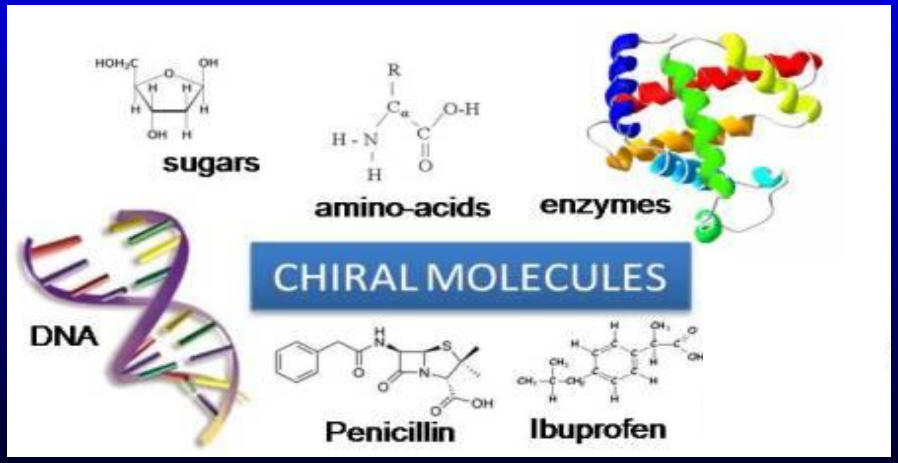




The homochirality of the building blocks of life (DNA, sugars, amino acids) is unexplained







Biological homochirality:
L-amino acids and D-sugars

Origin ?

P-breaking mechanism

exclude EM interaction

weak interaction ? No, too weak

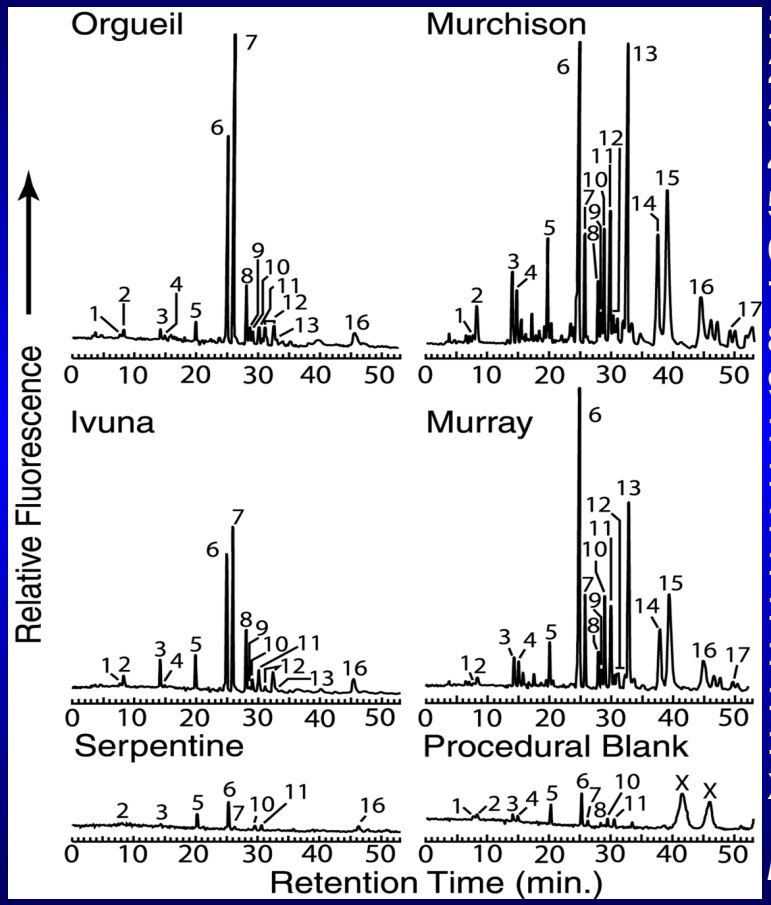
a chemical reasoning

bifurcation when big chain polymers form ?

Amino acids found in meteorites, with a preferred chirality

Excess in one mirror image

7-9% up to 60%



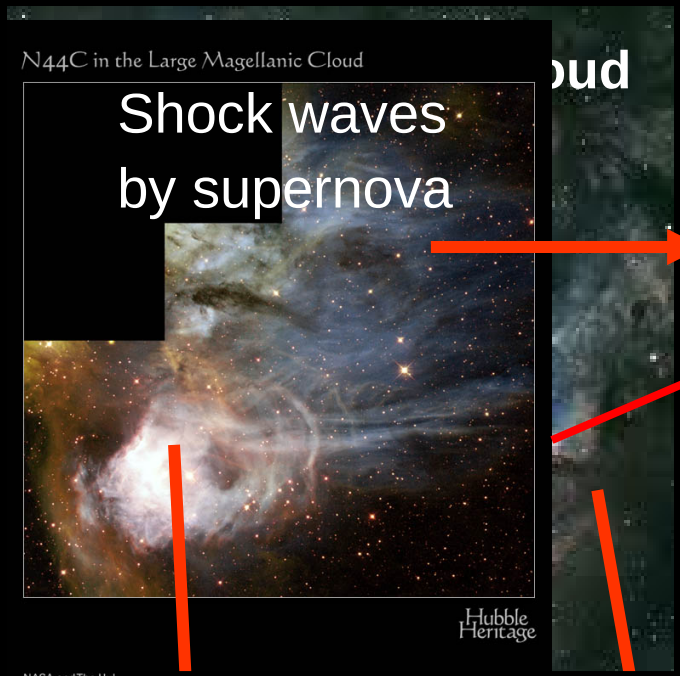
1 D-Aspartic Acid
2 L-Aspartic Acid
3 L-Glutamic Acid
4 D-Glutamic Acid
5 D,L-Serine
6 Glycine
7 β-Alanine
8 γ-Amino-*n*-butyric Acid
9 D,L-β-Aminoisobutyric Acid
10 D-Alanine
11 L-Alanine
12 D,L-β-Amino-*n*-butyric Acid
13 α-Aminoisobutyric Acid
14 D,L-α-Amino-*n*-butyric Acid
15 D,L-Isovaline
16 L-Valine
17 D-Valine
X: unknown

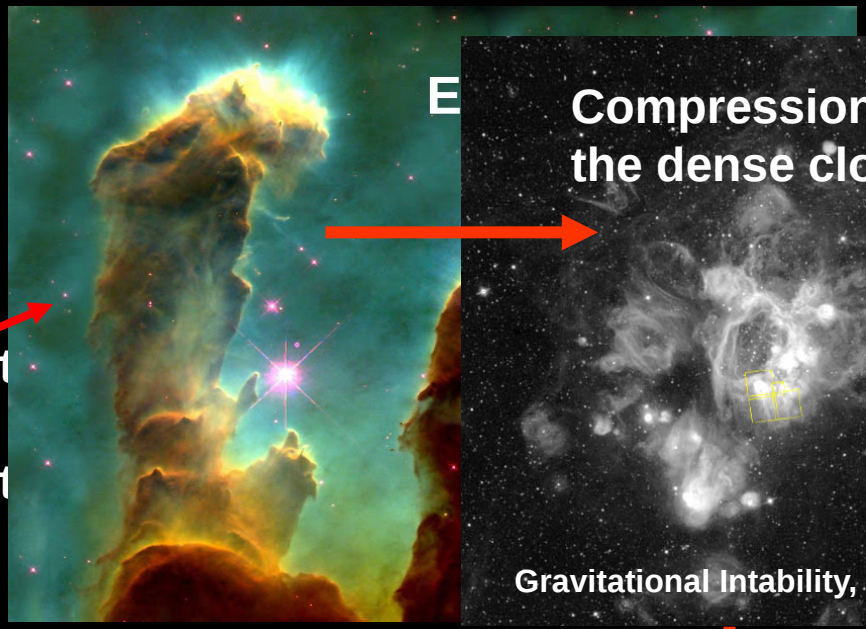
Ehrenfreund et al. 2001

Influence of a chiral cosmic perturbation ?

How amino acids formed in a cosmic context ?

History of a meteorite linked to interstellar Ices



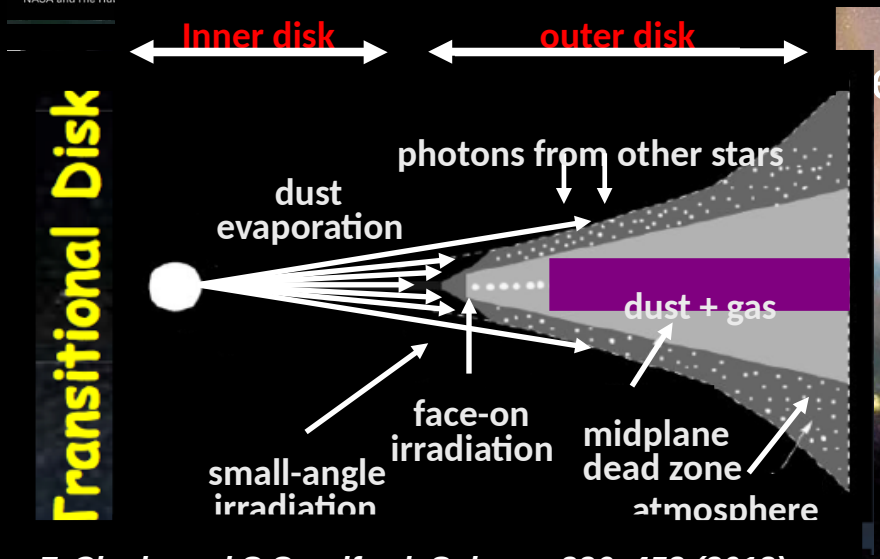


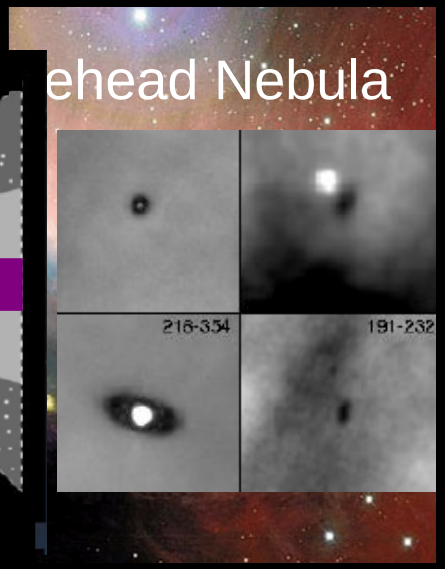
Compression of the dense cloud

Gravitational Intability, turbolence

Stars formation

… in the IR

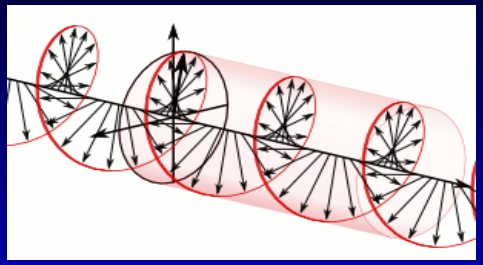


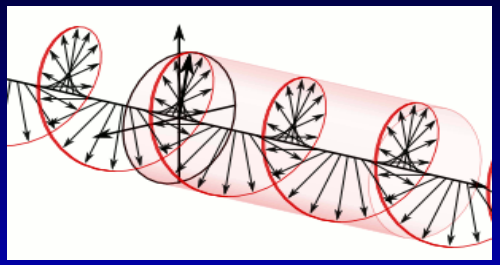


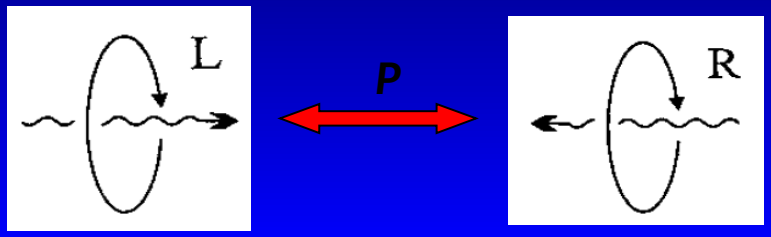
F. Ciesla and S.Sandford, Science 336, 452 (2012)

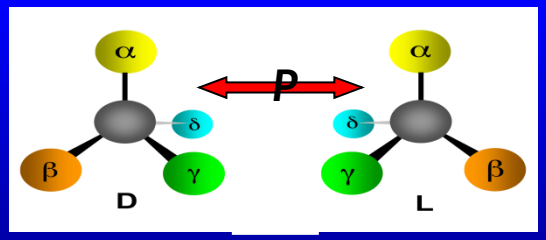
P-breaking by interaction with chiral perturbations:

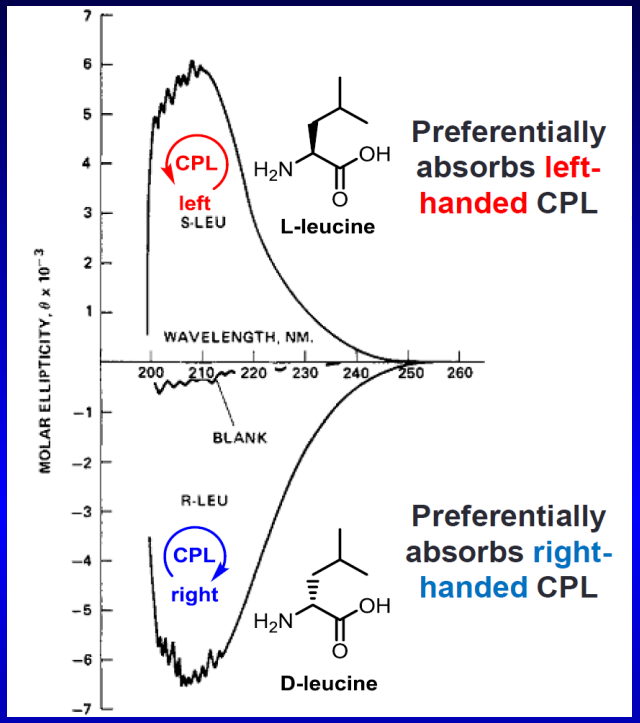
circularly polarized light (CPL) by close-by young stars







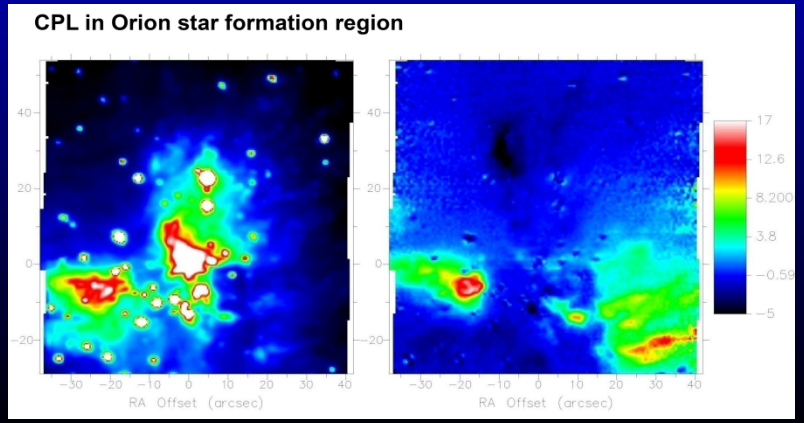




Cat's nebula 32% (IR), quadrupolar pattern,
Orion star formation region
O stars: *X-ray polarimetry*
black hole@center of our galaxy sgrA* (Radio)

Kwon et al. , Astrophysical Journal Letter 765, L 6 (2013)
Bailey et al, Science 281, 672 (1998)
Sudnik et al, AIP Conf. Proc. 1429,114 (2012)
Munoz et al., The Astrophysical Journal 745, 115 (2012)

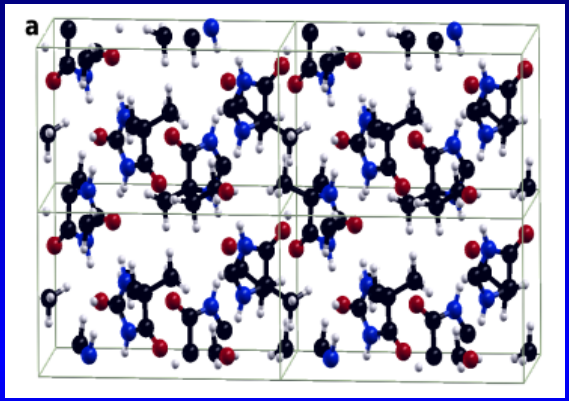
OUR LOCAL REGION: excess of right CPL



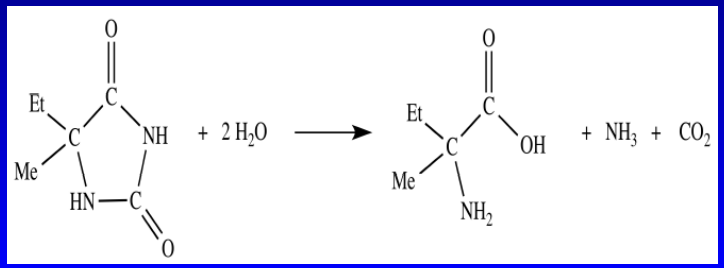
Imagine a “cold - warming phase - back to cold” scenario:

from precursors in molecular clouds to amino acids in outer-disk small bodies

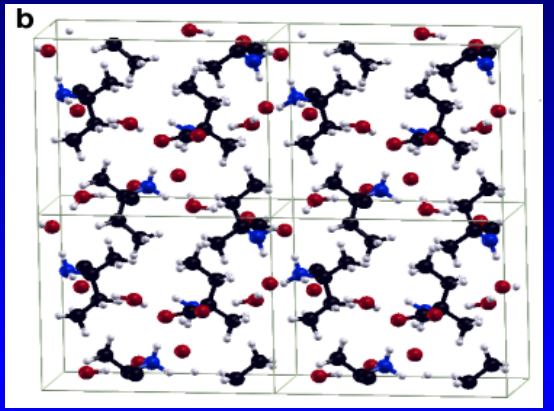
1) precursor, cold environment
5-ethyl-5-methylhydantoin



2) warming phase,
formation of the amino acid



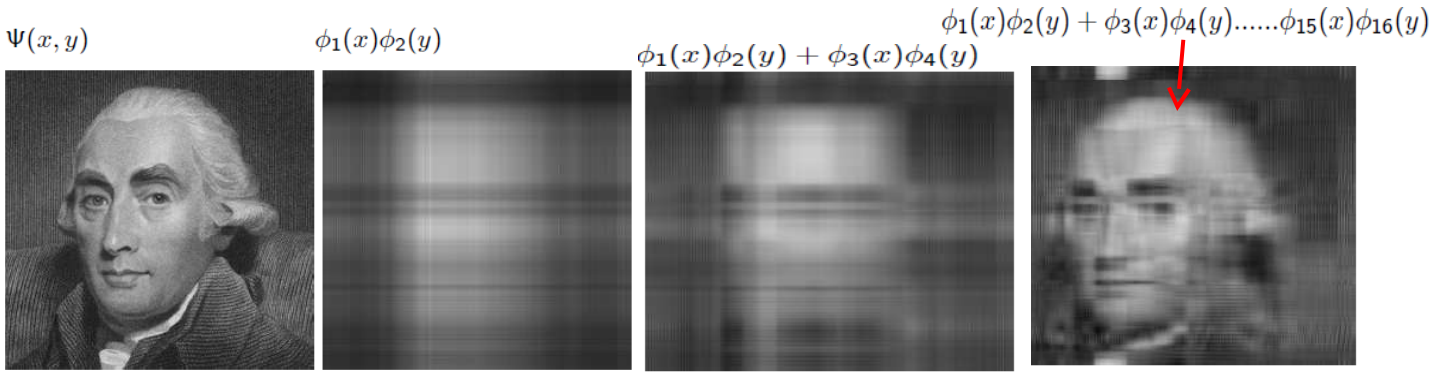
3) Isovaline,
recondensation within ice



Search for strong peaks in the difference of absorption for left and right circular polarization , in correspondance of energy needed to break specific C-C bonds

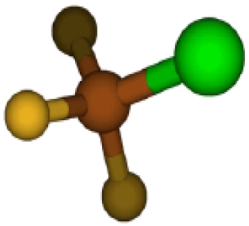
Which theoretical approach ?

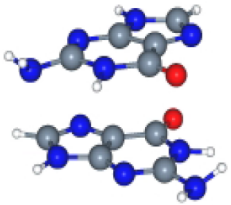
Wave-function approaches : unpractical in solids

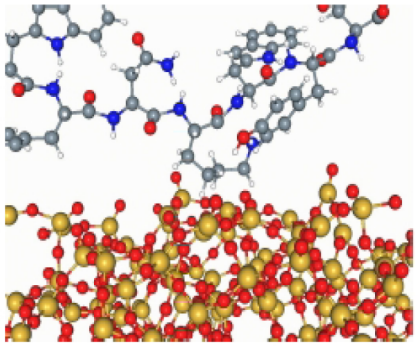


Propagators, Density –based approaches

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, .., \mathbf{r}_N, t) \longrightarrow G(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) \longrightarrow \rho(\mathbf{r}, t)$$

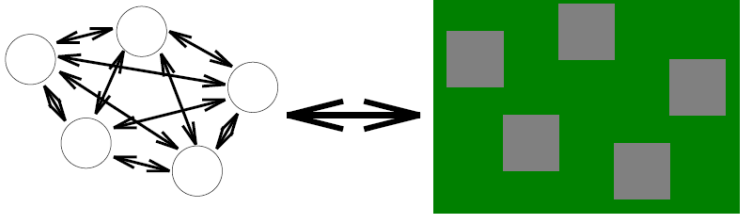






Time Dependent Density Functional Theory (DFT)

- allows dynamics and short range/long range correlations



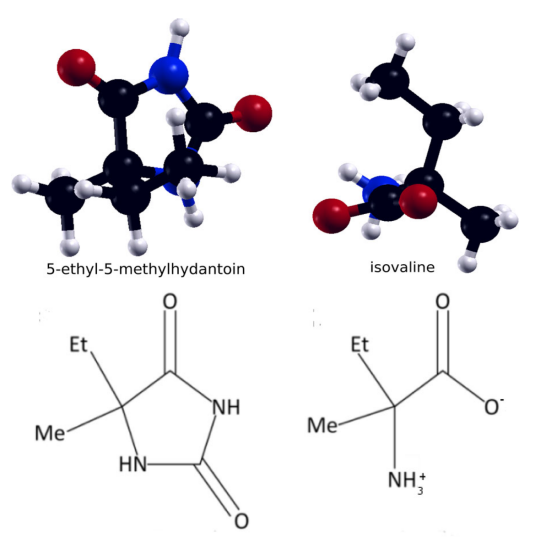
IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER
J. Phys.: Condens. Matter **24** (2012) 233202 (11pp) doi:10.1088/0953-8984/24/23/233202

TOPICAL REVIEW

Time-dependent density-functional theory in massively parallel computer architectures: the OCTOPUS project

Xavier Andrade[1], Joseba Alberdi-Rodriguez[2,3], David A Strubbe[4,5], Micael J T Oliveira[6], Fernando Nogueira[6], Alberto Castro[7], Javier Muguerza[3], Agustin Arruabarrena[3], Steven G Louie[4,5], Alán Aspuru-Guzik[1], Angel Rubio[2,8] and Miguel A L Marques[9,10]

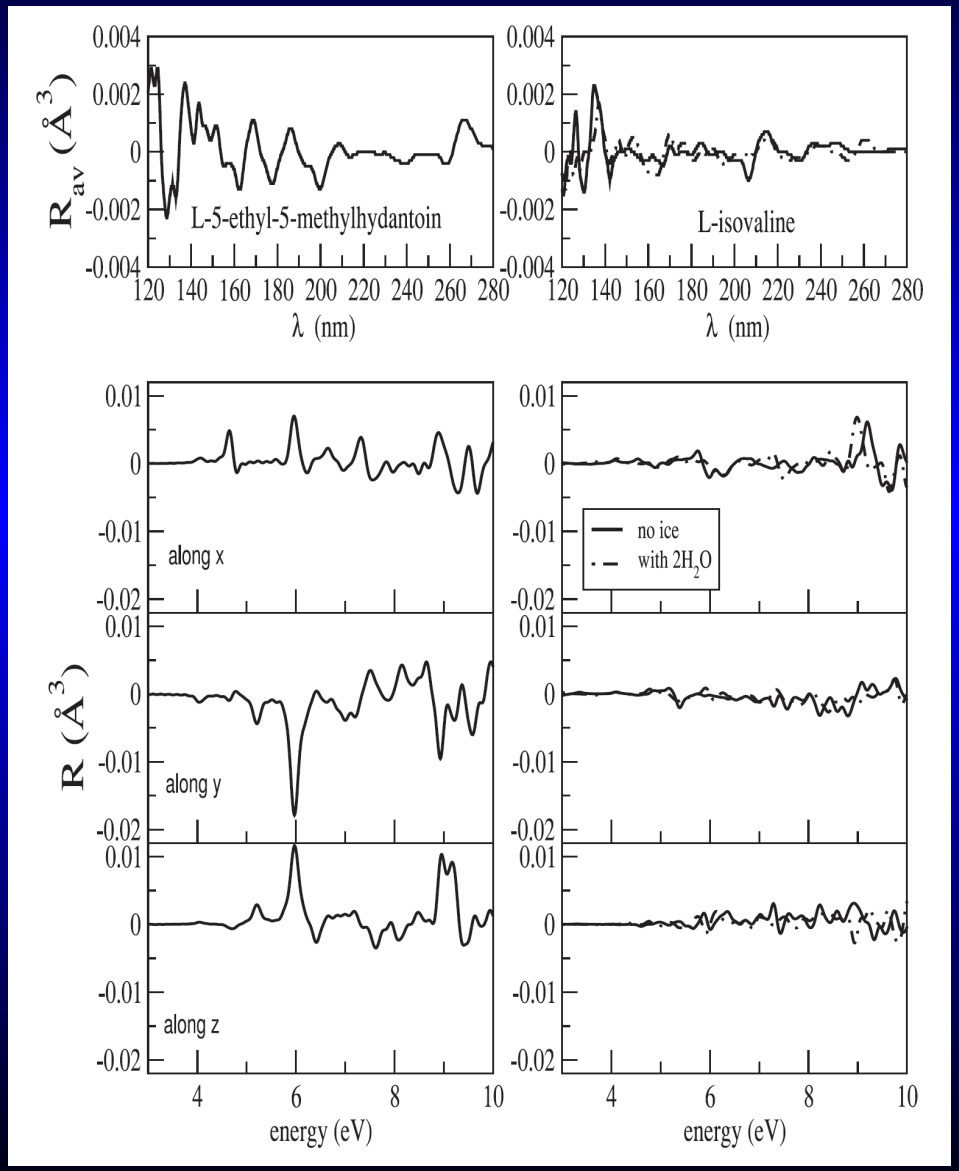
Results



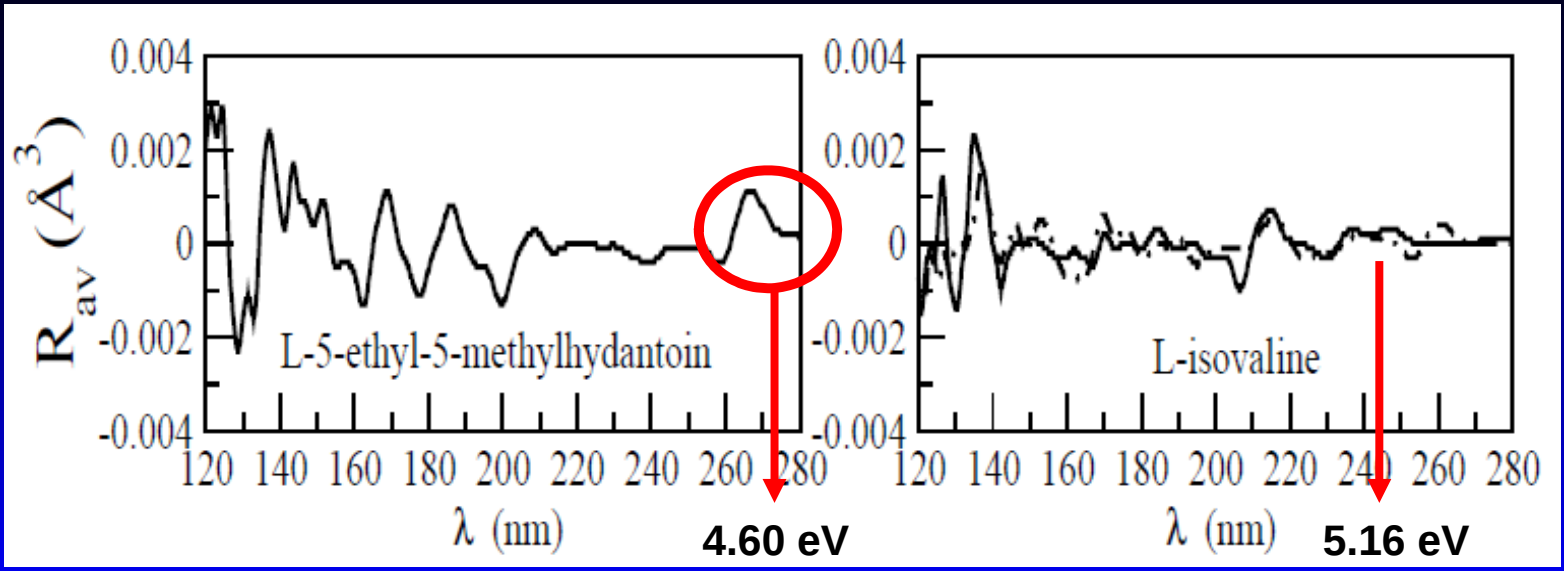
Strong directional dependence on the incidence direction of the light

No big influence of surrounding ice, agreement with film of isovaline

Takahashi J.-I. et al., 2009, Int. J. Mol. Sci., 10, 3044



FDP *et al., MNRAS 2014*



Peaks for the precursor are overall stronger in a region for selective C-C breaking

Important role of the precursors

In agreement with suggestions from Pizzarello et al, 2012, PNAS USA, 109, 11949

The Vacuum UV region is characterized stronger features

The Vacuum UV CPL light would constitute a P-breaking perturbation inducing a certain asymmetry in the two mirror images for both systems

FDP *et al., MNRAS 2014*

Information-theoretical content of the precursor and the amino acid

Fisher-Shannon Complexity

$$C_r(\mathrm{FS}) = I_r \cdot J_r$$

$$I_r = \int \rho(\mathbf{r}) |\vec{\nabla} \ln \rho(\mathbf{r})|^2 \, \mathrm{d}^3\mathbf{r}$$

$$J_r = \frac{1}{2\pi e} \exp\left(\tfrac{2}{3} S_r\right)$$

$$S_r = -\int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d^3\mathbf{r}$$

Departure of the probability density from disorder

Power Entropy ⊔ Shannon Entropy: measurement of the randomness of the probability density (measure the departure from localizability)

	#ELECTRONS	HARDNESS	C(FS)
amino acid	52	0.18	230
precursor	64	0.25	440

Please check R. Esquivel, PCCP 2010 for definitions

Future Plan

Effect of turbolence

Evaluating the time evolution of complexity (during the chemical reaction while interacting with water)

Thank you !