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Mathematical Studies on Structural Chemistry

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Abstract. The trans-disciplinary advantages of utilizing both mathematical developments and new chemical knowledge in structural chemistry, where this specific field involves fundamental physical, specifically, quantum physical fetures of molecular structures, are providing the basis for new research studies under the present project "Mathematical Studies on Structural Chemistry". These studies include some relevant biochemical and even medicinal chemistry problems, in part conneted to the earlier project of 2016, on cataract formation in the human eye caused by chirality changes in the L to D transformations of Aspartic Acid, and also studies focusing on the general patterns of such trans-disciplinary research fields, where components of the mathematical background, as illustrated by underlying principles in structural chemistry, serve as analogies for several of the currently undergoing developments in a far broader sense. Some of the principles observed in the above area of the overlap between mathematics and structural chemistry, also appear as valid in many current, far more general scientific and even more general human activities, as caused by the unprecedented interconnectedness brought about by the internet, that is the main factor of the highly accelerated changes in science, humanities, even art, as well as economy, providing a new level of integration of both intellectual and technical advances in society. Based on these principles, within this new research project, two specific studies have been started.

Keywords: Mathematical Tools for Structural Chemistry, Chirality and Symmetry Deficiency Measures and the HolographicTheorem, L-to-D Transformations of Amino Acids, Fractals and Fuzzy Sets from Molecules to Society, Analogies on Differing Levels of Organizations

1. Subject of the Report:

Research projects report for the Invited "Distinguished Visiting Professor" Visit of Prof. Paul G. Mezey, Canada Research Chair in Scientific Modelling and Simulation, Memorial University, St. John's, NL CANADA
Invitation by the Kyoto University International Research Unit of Advanced Future Studies, for a one-month visit as Distinguished Visiting Professor, in charge of "Mathematical Studies On Structural Chemistry", to be carried out in collaboration with of Professor Masatoshi Murase, at the Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto, Japan, June 1 – June 30, 2017.

2. Introduction

Motivated by the trans-disciplinary projects of Professor Masatoshi Murase (see, for example, Murase 2014, Murase 2015, and Murase 2017, and references therein), and in part the advances by Professor Noriko Fujii in the study of Aspartic Acid racemization in the process of cataract formation in the eye (see, for example, Fujii 2012, Sakaue 2015, and Sakaue 2017, and references therein), at the invitation of the International Research Unit of Advanced Future Studies, Yukawa Institute for Theoretical Physics of Kyoto University in the period of 2017 June 1 to June 30, the research project on **"Mathematical Studies On Structural Chemistry"** has been initiated, in part also continuing some of the initiatives of last year's project on "Local and Global Chirality Measures of Natural Amino Acids". The early developments already progressed far enough during that one-month period to be able to state that they will serve as the basis of two journal publications, in part also connected to two other publications, based on last year's projects, near completion and submission. The two main topics of the current Research Project are the following:

Topic 1. Mathematical treatment of the interrelations of the local shape, symmetry deficiency measures, and chirality measures of individual molecules and the alignment of surrounding molecules.
The study of Topic 1 has its focus on the study of interrelations among properties which are relevant to local interactions, such as those present within a single molecule, and those involving more global types of interactions, such as those among a set of molecules. Analogies with more complex systems, such as biological systems, and even society, are emphasized.

Topic 2. Combining Fractals and Fuzzy Set Theory in Studies on Molecular Structure and Analogies for Studies of Other Sciences, Humanities, Economy, and Society.
Studying Topic 2 is the more trans-disciplinary project, as at the outset, it involves two rather different branches of mathematics, and applies them to chemical, as well as to more complex systems.

The location of the research invitation for the project „Mathematical Studies on Structural Chemistry", has been the highly motivating environment of the home institute of Prof. Masatoshi Murase, the International Research Unit of Advanced Future Studies, at the Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto, Japan

3. Related Conference Participations and Lecture Presentations:

I participated in the symposium and I took part in the plenary discussions as a member of the audience at the following Symposium:

The Kyoto Symposium 4, "The Kyoto Manifesto for Global Economics", Doshisha University, Kyoto, 2017 June 4, an international conference on the role of science and humanities in the future of global economy.

My discussion with the panel and the audience involved pointing out the huge gap between the current revolutionary possibilities of internet-based communication and

the actual lagging behind with the efficient utilization by science, art, economy, and society in general.

In addition, during this one-month visit, two lectures have been presented by Prof. Paul G. Mezey.

Lecture 1:
Paul G. Mezey: "A Fuzzy Set Approach to the Complexity of Unexpected Consequences in Chemistry and in Society".
The essential message of this presentation: Both complexity and fuzziness can be treated by mathematical tools.

Complexity can be treated by the tools of information theory. The quantity of information required for a complete description is a measure of complexity.
Fuzziness can be treated by fuzzy set theory, introduced by Professor Lotfy Zadeh, of the University of Berkeley.
Both of these tools are applicable not only in Chemistry, but in a wide range of sciences and intellectual activities.

Presented at the
Transdisciplinary Mie-Symposium 2017, "Origins and Evolutions of Complexity"
Date: June 17 -18, 2017, Place: Mie Prefectural Museum

Co-organized by
Mie Prefectural Museum
and
International Research Unit of Advanced Future Studies (IRU-AFS). Kyoto University
Co-chairs:
Terufumi Ohno (Mie Prefectural Museum), and
Masatoshi Murase (IRU-AFS, Kyoto University)

Lecture 2:
Paul G. Mezey: "The way I see the FUTURE"
Subtitle: "Trying to Serve the Future Better by More Trans-disciplinary Connections to Biology, other Sciences, Society, History, Poetry, Visual Arts, and Music"

Presented at the
Yearly Activity Summary of the International Research Unit of Advanced Future Studies, Yukawa Institute for Theoretical Physics, Kyoto University
Date: June 24, 2017, Place: International Research Unit of Advanced Future Studies, Yukawa Institute for Theoretical Physics, Kyoto University.

4. Initial Research Progress with Topic 1:

Topic 1. Mathematical treatment of the interrelations of the local shape, symmetry deficiency measures and chirality measures of individual molecules and the alignment of surrounding molecules.

The study of Topic 1 has its focus on the structural chemistry consequences of local shape changes of individual molecules, as caused by alignment changes of neighboring molecules in their surroundings. This project, although also connects to the chirality changes studied in last year's project, is far more general, based on a specific application of the Holographic Electron Density Theorem (Mezey, 1999)

to a set of molecules, instead of just to individual molecules. At the same time, the findings already show the possibilities of utilizing these results as analogies in far broader scientific and even social investigations, where the individual entity (a molecule in the original case), and its relations with its surroundings (additional, nearby molecules in the original case), for example, in studies of the behaviour of single cell within a biologicl tissue, or even the internal workings of an industrial company as influenced by the interctions of competing companies within an economic system. Whereas the actual forces and the types of interactions are very different in in structual chemistry and in society, it can be vauable to recognize some of the analogies. Just as an electromagnetism experiment in a physics laboratory is very different form the weather pattern over a country, nevertheless, the same Maxwell equations describe both. Although the participting variables and the boundary conditions are very diferent, nevertheless, the set of equations, that is, the fundamental pattern of rules, are the same. In a similar sense, an appoximate „Holographic Theorem" is applicable far beyond chemistry, and provides motivation for serching for new principles and relations in very different fields as well.
One manuscript is in preparation.

5. Initial Research Progress with Topic 2:

Topic 2. Combining Fractals and Fuzzy Set Theory in Studies on Molecular Structure and Analogies for Studies of Other Sciences, Humanities, Economy, and Society.

Studying Topic 2 is the more trans-disciplinary project involving the the two Topics, where two branches of mathematics, the theory of Fractals and the formalism of Fuzzy Set Theory are combined, initially, to approach some complex structural chemistry problems, but also providing a somewhat general pattern in dealing with the interrelation of different levels of detail when describing a phenomenon, and the somewhat fuzzy way the actual levels of these fractals are defined in most scientific, philosophical, artistic, industrial, economy-related, and society problems.
One manuscript is in preparation.

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