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Fuji Zhang's Work in Mathematical Chemistry

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The logo of the International Academy of Mathematical Chemistry (IAMC) is a hexagon composed of two halves, in which one contains the letter C, and the other contains the letter M. When reading the autobiographical notes of Professors A. T. Balaban and M. Randić, we found that they belong to the same half in the two, and that Professor Fuji Zhang belongs to the other half as a mathematician. Professor Zhang's work showed that mathematical chemistry is beneficial not only for chemistry but also for mathematics. To celebrate Professor Zhang's 80th birth day, we write this article, giving a brief description of his work in mathematical chemistry and his work stimulated by mathematical chemistry, in related branches of mathematics including combinatorics, graph theory, and knot theory, as well as in statistical physics.

Zhang began to be interested in natural sciences since his childhood. After graduation from high school in 1954, he was enrolled in the department of mathematics in Beijing Normal University and was trained as a mathematician and teacher. For political reason, Zhang was treated unfairly for two decades since 1958 until the so called Cultural Revolution ended completely and China started the reform and began to open its door to the world (refer to [1] for details). Zhang's misfortune and varied career reflects the fate of many Chinese intellectuals in his age.

In the early 1970s Zhang was first exposed to mathematical chemistry by chance when one of his relatives living abroad sent him some literatures in mathematics and sciences. Before that, Zhang had been working in the field of queuing theory. In 1976 he read a paper of Au-Ching Tong and Yuan-Sun Jiang [2] published in the journal Science in China (*Scientia Sinica*). In that paper the authors Tong and Jiang provided two recurrence formulas to compute the characteristic polynomial of a weighted graph which can be used to deal with the orbital of a molecule with carbon-heteroatom bonds, but they did not prove their formulas. Then Zhang worked out a proof of the recurrence formulas and published the result in the same journal [3], which is his first paper in mathematical chemistry. Later on, when Zhang had opportunity to get access to resources with richer foreign math literatures, he found that in the case of graphs that correspond to the molecules with only carbon-carbon bounds, similar results had been obtained by A. J. Schwenk [4]. After Zhang published his first paper in mathematical chemistry, he received a letter from Dr. Ivan Gutman requesting an offprint of the paper. And at the same time, Dr. Gutman kindly sent Zhang lots of his publications from Yugoslavia, which greatly stimulated Zhang's research interest in the field of mathematical chemistry.

In 1981, after Zhang was invited to join the department of mathematics in Xinjiang University, he organized a seminar on graph theory and its applications. The participants were his young colleagues and graduate students in the university. Some of the seminar participants were interested in mathematical chemistry, and the other participants mainly worked in other topics in graph theory and the theory of probability. In last century Zhang's main collaborators in mathematical chemistry were Rongsi Chen, Zhibo Chen, Xiaofeng Guo, Xueliang Li, Heping Zhang and Maolin Zheng.

Zhang's first foreign collaborator is Dr. Gutman. In 1978, the concept of the energy of a graph introduced by Gutman inspired Zhang to join the research on partial orderings of graphs. Two joint papers [5,6] were published by Gutman and Zhang on the ordering of graphs with respect to their matching numbers and coefficients of their characteristic polynomials respectively. In fact, at that time Zhang published most of his papers in Chinese journals, just as other Chinese mathematicians did. Zhang kept his interest in the extreme energy of

molecular graphs. In his joint papers [7-8] with H. Li, they proved two conjectures of Gutman on extreme acyclic conjugated molecules, and they proposed some new approaches to solve the extreme problems. Many years later, Zhang returned to study the energy of aromatic polycyclic compounds (in the foregoing years researchers only concentrated on trees, unicyclic graphs and bicyclic graphs). Zhang solved the extreme energy problem of hexagonal chains and double hexagonal chains with co-authors [9-12]. A complete account of main results on the graph energy can be found in the monograph [13] by X. Li, Y. Shi and I. Gutman, in which some other work done by Zhang and his students W. Yan and J. Ou are included. In Zhang's joint paper with Z. Chen and I. Gutman [14], they extended the concept of S, T- isomers introduced by O. E. Polansky, and proved some topological properties. In [15] Zhang and Z. Chen introduced two types of new S, T- isomers and proved some topological properties of them. Afterwards, some novel S,T-isomers and generalizations were introduced and studied, see V. I. Elkin [16] , Zhang and Z. Chen [17], H. Zhang [18], X. Li [19], X. Li and Y. Liu [20], X. Li and S. Zheng [21], Y. Yang and D.J. Klein [22]. It is worthy to mention that the Clar covering polynomial defined by H. Zhang and F. Zhang was used as a novel tool to conveniently compare the resonance structure counts of some S,T-isomers.

In 1984, Zhang, X. Guo and R. Chen, inspired by the mathematician Horst Sachs' work, obtained a necessary and sufficient condition for the existence of perfect matching in a hexagonal system, when they had no knowledge of the fact that the same result had been obtained by A. V. Kostochka independently. Some historical notes were provided along with some powerful algorithms in [23]. Later, Zhang and Guo [24] extended these results to helicenes. R. Chen et al. [25] obtained a necessary and sufficient condition of the existence of perfect matchings in coronoid hydrocarbons, an algorithm for recognizing Kekule structure in benzenoid and coronoid and coronoid systems had been obtained by Zhang and Lin [26]. H. Zhang and F. Zhang [27] obtained a similar result for square lattices.

In 1980s many researchers were interested in searching for concealed non-kekulean benzenoid hydrocarbons, namely the non-kekulean benzenoid hydrocarbons with the same number of vertices in two different colors (see [28] and references cited therein). Zhang and

Guo found that they can use the necessary and sufficient condition of the existence of perfect matching in a hexagonal system to get the needed graph constructions in the proof for some enumeration results of concealed non-kekulean benzenoid hydrocarbons mathematically rather than using brute force computer search. They constructed concealed non-Kekulean benzenoid hydrocarbon up to 13 hexagons [29-30]. Furthermore, Guo and coauthors constructed the concealed non-kekulean benzenoid hydrocarbon with 14 hexagons [31]. The results answered a question of S. J. Cyvin, and confirmed the results of Dusseldorf-Zagreb group obtained by computer search [28]. Many years later R. Chen and his coauthor determined all concealed non-Kekulean coronoid hydrocarbons with minimum number of hexagons [32].

Another paper of Zhang joint with R. Chen, X. Guo and I. Gutman showed that if x, y and z denote the number of mutually parallel double bonds in a Kekule structure of a benzenoid hydrocarbon respectively then all Kekule structure in this hydrocarbon have the same (x,y,z) – triple. This invariant can be used to determine the Clar number (the maximum number of independent resonant hexagons in a benzenoid hydrocarbon), which were previously only observed without proof [33]. Zhang and Guo [34] characterized this invariant of the benzenoid hydrocarbon, and together with R. Chen and Gutman [35] they characterized benzenoid hydrocarbons whose (x,y,z)-invariants have x=1 and 2. In this century, stimulated by the study of grapheme, Yan, Yeh and Zhang [36] and Ren, Zhang and Qian [37] applied this result to the dimer problem in statistical physics. They showed that for the honeycomb lattice whose free energy per-dimer equals zero, if we consider their (x,y,z) invariant, their free energy per-dimer is non-zero. Furthermore, W. Yan and Z. Zhang introduced the concept of energy of graph to statistical physics [38].

In the book by Gutman and S. J. Cyvin [39], they cited the result of Zhang and R. Chen [40] on the necessary and sufficient condition for benzenoid hydrocarbons to have equal number of Kekule structures and generalized Clar structures. Since then Cyvin often mailed his books and papers to Zhang from Norway and discussed problems with Zhang, Guo and R. Chen by land mails (since there was no internet available yet at that time of last century.) Professor D. J. Klein also mailed his publications to Zhang from the USA. In the seminar led by Zhang at

Xinjiang University, the participants frequently discussed the works of Gutman, Cyvin, and Klein, which resulted in pleasant international collaborations.

In 1991 Zhang and Guo visited the University Trondheim in Norway, where they did a lot of polyhex enumeration research with Cyvin and his team. Some results are presented in a book edited by Gutman [41]. Their other results can be found in [42-46]. The topic of enumeration always attracts Zhang's interest. Quite a few years later Zhang solved some enumeration problem in chemistry and statistical physics [47-50] with J. Qian, K. Deng, et al. Zhang also considered the construction of regular single coronoid hydrocarbons with R. Chen based on a result of Zhang and M. Zheng [51]. Their results are included in a book (chapter 8) of S. J. Cyvin et al. with R. Chen and Zhang being co-authors [25]. In the case of multiple coronoid hydrocarbons, some further results had been given in [52,53]. Later, Zhang, R. Chen and S. J. Cyvin gave a complete solution of Hosoya's mystery concerning the coincidence between the characteristic polynomial and the polynomial of Kekule structure count of a primitive coronoid hydrocarbon [54].

In [55] F. Harary and Klein defined an edge of a graph to be forcing edge if it belongs to exactly one perfect matching. Zhang and X. Li [56] determined the hexagonal systems with a forcing edge. X. Li [57, 58] further defined the concept of forcing single edge. These concepts have been developed as forcing number and anti-forcing number of perfect matchings in general graphs [59-61]. Soon after Zhang solved some problems in mathematical chemistry with his students and foreign scientists, he found that not only he can prove or disprove something proposed by chemists in mathematical chemistry, but he can also further introduce some new concepts in mathematical chemistry reasonably. Furthermore, he realized that some results in mathematical chemistry can inspire him to obtain some new results in graph theory, combinatorial computation, and even in knot theory and statistical mechanics. The main concepts introduced by Zhang and his students are: Z-transformation graphs of hexagonal systems and plane bipartite graphs; k-resonance in hexagonal systems (i,e., benzenoid systems, the molecular graphs of benzenoid hydrocarbons), open-ended carbon nanotubes, toroidal

polyhexes, or plane bipartite graphs; k-cycle resonant graphs in general graphs; and Clar covering polynomial (Zhang-Zhang polynomial) of hexagonal systems.

In 1988 F. Zhang, X. Guo and R. Chen [62-64] introduced the "Z-transformation graph" (denoted Z(H)) of perfect matchings of a hexagonal system H: the vertices of Z(H) are the perfect matchings of H and two perfect matchings are joined by an edge provided they only differ in one hexagon (in other words, the two perfect matchings can be obtained from each other by rotating one resonant hexagon in H). They deduced basic mathematical properties of Z(H), for example, Z(H) has at most two end vertices, and they characterized the hexagonal systems H whose Z(H) has one and two end vertices, respectively. In chemistry, this idea originated from Herndon's resonance theory [65] put forward in 1973，and was introduced by W. Gründler [66,67] but no corresponding mathematical results followed. A somehow similar transformation (called the sextet rotation, rotating a kind of resonant hexagons in a perfect matching of a hexagonal system H simultaneously) had been employed to define a directed graph D(H) by Ohkami, Motoyama, Yamaguchi, Hosoya, and Gutman in their joint paper [68] to study the hierarchical structure among the perfect matchings of a hexagonal system H. They proved that D(H) has the structure of a directed tree with a root for the special case when H has no three hexagons with a vertex in common. In the same paper they pointed out that they believe the result is also valid for general hexagonal systems but a rigorous proof has not been found. A few years later, this conjecture was proved by Z. Chen in [69] where he also established further result for generalized hexagonal systems (with "holes" inside). This inspired some further investigations of the lattice structure of the Z-transformation graph.

The concept of Z-transformation graph was extended naturally to general plane bipartite graphs by H. Zhang and F. Zhang [70]. In the cases of hexagonal system and polyomino it was redefined many times under different names. It was redefined and called resonance graph by Randic [71,72] in which it is shown that the leading eigenvalue of the resonance graph is correlative with the resonance energy of the benzenoid. In 2003 J. C. Fournier [73] used the name "perfect matching graph" for this graph in investigating domino tiling spaces of Saldanha and Casarin. To date rich theoretical results have been made in this field by several

research groups. In particular, the distributive lattice structure [74,75] and median property [76,77] on Z-transformation graph of plane bipartite graphs have been established. Its nature can be explained in many ways from chemical resonance to mathematical cycle space, distributive lattice and median property. More details can be seen in the survey by H. Zhang [78].

Let G be a benzenoid system, an open-ended nanotube (tubule), or a toroidal polyhex with at least k disjoint hexagons. The graph G is said to be *k-resonant* or *k-coverable* [79] if, for $1 \le t \le k$, any t disjoint hexagons of G are mutually resonant, that is, there is a Kekule structure M of G such that each of the k hexagons is an M-alternating hexagon. The 1-resonant benzenoid systems were first introduced by Gutman [80], where a sufficient condition for a benzenoid system to be 1-resonant was also given. Some necessary and sufficient conditions for a benzenoid system to be 1-resonant (resp. normal or elementary -- each edge is contained in a Kekule structure) had been given by F. Zhang and R. Chen [81]. Among those the most elegant one is "a benzenoid system is 1-resonant if and only if its boundary is a resonant cycle". The statement had been extended to polyomino [82] and more general weak elementary plane graphs [70]. Later on, Zhang and M. Zheng [83] gave a similar characterization for 1-resonant generalized benzenoid systems. Zhang further proposed the concept of k-resonant benzenoid systems in the graph theory seminar at Xinjiang University. Then M. Zheng [84] determined the 2-resonant benzenoid systems and further gave a pretty result for k-resonant benzenoid systems with $k \ge 3$ in [85]: the 3-resonant benzenoid systems are also k-resonant for any integer $k \ge 4$ and can be constructed by combining three types of benzenoid systems as building bricks. He also gave the lower bound of the Clar number of a k-resonant benzenoid system for $k \ge 3$. R. Chen and Guo [86], K. Lin and R. Chen [87] generalized Zheng's results to generalized benzenoid systems. S. Liu and H. Zhang [88] further got similar results in some class of 2-connected plane bipartite graphs in which every face has size at least six and every inner vertex has degree 3 while the others have degree 2 or 3.

Zhang and L. Wang [89] first investigated k-resonance of tubules. They gave the construction method of k-resonant tubules for k=1 and $k \ge 3$, where the construction method of 1-resonant tubules is due to a method of constructing 1-resonant plane bipartite graphs given

in H. Zhang and F. Zhang[70]. In addition, Zhang and L. Wang [89] gave the lower bound of Clar number of k-resonant tubules for k ≥ 3. For *k*-resonant toroidal and Klein-bottle polyhexes, complete characterizations were given in several papers, see W. C. Shiu, P. C. B. Lam, and H. Zhang [90] , D. Ye and H. Zhang [91], W. C. Shiu and H. Zhang [92], and Q. Li, S. Liu, H. Zhang [93]. The k-resonance problem were further generalized to fullerenes and solved completely. For (4,6)-fullerenes (boron–nitrogen fullerenes), H. Zhang and S. Liu [94] showed that all (4,6)-fullerenes are 2-resonant and constructed all the 3-resonant B–N fullerene graphs, which are all k-resonant for any positive integer k. For (5,6)-fullerenes (carbon fullerenes), D. Ye, Z. Qi and H. Zhang [95] showed that every fullerene graph is 1-resonant and there are exactly nine 3-resonant fullerene graphs, which are also k-resonant for each k ≥ 4. They also proved that every leapfrog fullerene graph is 2-resonant. In general Kaiser et al. [96] showed that every IPR fullerene is 2-resonant and R. Yang and H. Zhang [97] gave a generalization. Finally, R. Yang completely characterized the 2-resoant fullerenes in her doctoral dissertation [98].

The concept of *k*-cycle resonant graphs was first introduced by X. Guo and F. Zhang [99], which is a natural generalization of the concept of *k*-resonant benzenoid systems. A connected graph *G* is said to be *k*-cycle resonant if, for $1 \le t \le k$, any t disjoint cycles in *G* are mutually resonant. Some properties and necessary and sufficient conditions of *k*-cycle resonant graphs and planar *k*-cycle resonant graphs were given in [99-105].

A Clar cover of G is a spanning subgraph of G in which each component is either a hexagon or a single edge. In 1996 H. Zhang and F. Zhang [106] formally introduced the concept of Clar covering polynomial of a hexagonal system as a counting polynomial of Clar covers of a benzenoid hydrocarbon, which includes more information about resonant structures, such as the Clar number, Clar structure count, Kekule structure count and the first Herndon number. Some general reduction computations have been developed. H. Zhang, F. Zhang, and Y. Liu [107] first revealed a relevance of the Clar covering polynomial with the resonance energy of benzenoids. Some connections with sextet polynomials and chromatic polynomials are also revealed by Zhang and his co-workers [108,109]. F. Zhang and H. Zhang showed that the

coefficients of the first half terms with higher degrees in a Clar covering polynomial form a strictly decreasing sequence, and they proposed a conjecture that the coefficients of the Clar covering polynomial of a hexagonal system form a unimodal sequence. This conjecture has not been resolved yet to this day. In a series of papers [110-115] Gutman et al. established some connections of the Clar covering polynomial with the resonance energy and renamed this polynomial as ``Zhang-Zhang polynomial". Recent work [116] showed that the Clar covering polynomial of a hexagonal system H coincides with the cube polynomial of the Z-transformation graph Z(H). The cube polynomial of a median graph was introduced by B. Brešar, S. Klavžar and R. Škrekovski [117]. C.P. Chou et al. [118-120] developed some methods including automatic computation to obtain the Zhang-Zhang polynomials for many types of benzenoids. More details of the works on the Clar covering polynomial can be seen in the survey [121].

It is well known that in the study of mathematical chemistry, three main branches of mathematics are widely applied: combinatorics, group theory and topology (knot theory in particular). In 1961 Frisch and Wasserman [122] first synthesized a pair of linked rings, known as the Hopf link in knot theory and as catenanes in chemistry. Since then many molecules in the form of knots, links and more general spatial graphs had been synthesized by chemists and biologists by the late 1980s. At that time there was the Jones revolution in knot theory in the field of mathematics. In the early 1990s Zhang began to have interests in knots and more general topology and made some preparations for future new research.

In 1994, Zhang was invited to join the department of mathematics at Xiamen University. While he continued to work in his former research fields, he strove to explore some new fields. In 2000, an eminent topologist Professor Boju Jiang of Peking University was invited to come to Xiamen University to give a series of speeches on knot theory. Jiang's speeches further motivated the combinatorics group of Xiamen University to enter this new field. From then Professor Zhang began to study some monographs on knots and pursued research in knot theory with his Ph.D student X. Jin, mainly using tools from graph theory.

They first studied the computation of the Jones polynomial of links formed from a graph by

replacing edges by parallel twists [123], reducing it to the chain polynomial of labeled graphs [124,125]. Then they generalized it to two kinds of twists, parallel or perpendicular [126]. Based on [123], Zhang and his Ph. D student W. Yang further reduced the computation to the chain polynomial of labelled cubic 3-polytopes [127]. Motivated by works in statistical mechanics, Zhang and Jin also studied the distribution of zeros of Jones polynomials and obtained the unit-circle theorem[128], i.e. the accumulation set of zeros of Jones polynomials of links under twisting is the unit circle and several isolated points. Finally X. Jin, F. Zhang, F. Dong and E. Tay solved the computational problem of the Jones polynomial of the general case: replacing an edge by a 2-tangle and in the same paper they proved that the zeros of Jones polynomials of links are dense in complex plane [129]. Then they turned to the more powerful 2-variable HOMFLY polynomial. In 1988 F. Jaeger constructed an oriented link L(G) from a plane graph G by substituting edges of G by clasps and built a relation between the HOMFLY polynomial of L(G) and the Tutte polynomial of G [130]. Next year L. Traldi considered four kinds of clasps and did the similar work [131]. In 2012, X. Jin and F. Zhang [132] generalized F. Jaeger and L. Traldi's works from clasps to general substitution of alternatingly oriented 2-tangles. This work was cited in the references of the recent monograph [133] about graphs on surfaces. In addition, X. Jin and F. Zhang further studied zeros of HOMFLY polynomial with one variable z fixed[134].

The above theoretical results on knots found applications[135-137] in quantizing and analyzing DNA polyhedra. In fact, before the works mentioned above, works on polynomials of polyhedral links, the mathematical model of DNA polyhedra had been done by H. Zhang, W. Qiu and their students G. Hu, X. Cheng and S. Liu etc [138-141]. Later, based on the results in [132] and [134], X. Cheng, Y. Lei and W. Yang [142] obtained the HOMFLY polynomial of the double crossover tetrahedral link which has 96 crossings. By applying the star-triangle transformation, M. Li, Q. Deng and X. Jin further obtained the HOMFLY polynomial of the double crossover hexahedral link [143] with 192 crossings.

As the research goes on and deepens, Professor Zhang always asks his students to think about some new questions. To conclude this paper let us mention the following three of his

questions. 1. How about invariants of links obtained from a graph by replacing a vertex of degree d by a d-tangle? Such invariants can be used to deal with protein polyhedra [144], whose several numerical invariants have been studied [145-148]. 2. How to define a spatial graph invariant so that we can use it to judge the topological chirality of spatial graphs in Euclidean 3-space? 3. How to understand our numerical results more deeply from the viewpoint of chemistry and biology?

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