

**Bih-Yaw Jin****Recent publications**

1. Chang, Yao-Wen; Jin, B.-Y.\* Theory of Charge Transport Through Molecular Junctions: From Coulomb Blockade to Coherent Tunneling *J. Chem. Phys.* **2014**, 141, 064111.
2. Varadwaj, Pradeep R.\*; Varadwaj, Arpita; Jin, Bih-Yaw\* Halogen Bonding Interaction of Chloromethane with Several Nitrogen Donating Molecules: Addressing the Nature of the Chlorine Surface  $\sigma$ -hole *Phys. Chem. Chem. Phys.* **2014**, 16, 19573-19589.
3. Fan, Yuan-Jia; Jin, B.-Y.\* From the “Brazuca” ball to octahedral fullerenes: Their construction and Classification, **2014**, *arXiv:1406.7058* [physics.atm-clus]
4. Varadwaj, Pradeep R.\*; Varadwaj, Arpita; Jin, B.-Y.\*, Significant Evidence of C...O and C...C Long-Range Contacts in Several Heterodimeric Complexes, Should One Refer Them as to Carbon Bonds and Dicarbon Bonds! *Phys. Chem. Chem. Phys.* **2014**, 16, 17238-17252.
5. Ai, Qing; Fan, Y.-J.; Jin, B.-Y.; Cheng, Y.-C.\*, An Efficient Quantum Jump Method for Coherent Energy Transfer Dynamics in Photosynthetic Systems under the Influence of Laser Fields, *New J. Phys.* **2014**, 16, 053033.
6. Shen, Yao; Ko, Hsin-Yu; Ai, Qing; Peng, Shi-Ming; Jin, Bih-Yaw\*, Molecular Split-Ring Resonators Based on Metal String Complexes. *J. Phys. Chem. C.* **2014**, 118, 3766–3773.
7. Shen, Yao; Jin, Bih-Yaw\*, Correspondence Between Gentile Oscillators and N-Annulenes. *J. Phys. Chem. A.* **2013**, 117, 12540-12545.
8. Huang, H.-C.; Shiung, K.-S.; Jin, B.-Y.; Tzeng, Wen-Bih\*, Rotamers of m-chloroanisole studied by two-color resonant two-photon mass-analyzed threshold ionization spectroscopy, *Chemical Physics*, **2013**, 425, 114-120.
9. Ai, Qing; Yen, Tzu-Chi; Jin, Bih-Yaw; Cheng, Yuan-Chung\*, Clustered Geometries Exploiting Quantum Coherence Effects for Efficient Energy Transfer in Light Harvesting, *J. Phys. Chem. Lett.* **2013**, 4, 2577-2584.
10. Chuang, C.; Fan, Y.-C.; Jin, B.-Y.\* Comments on Structural Types of Toroidal Carbon Nanotubes, *J. Chin. Chem. Soc.* **2013**, 60, 949-954.
11. Chang, Y.-W.; Jin, B.-Y.\* Self-Interaction Correction to GW Approximation, *Physica Scripta* **2012**, 86, 065301.
12. Huang, H.-C.; Jin, B.-Y.; Tzeng, W.-B.\* Two-color resonant two-photon ionization and mass-analyzed threshold ionization spectroscopy of o-chloroanisole, *J. Photochem. & Photophys. A: Chemistry* **2012**, 243, 73-79.
13. Chang, Y.-W.; Jin, B.-Y.\* Correlation Effects of  $\pi$  Electrons on the Band Structures of Conjugated Polymers using the Self-Consistent GW Approximation with Vertex Correction, *J. Chem. Phys.* **2012** 136, 024110.
14. Chuang, C.; Fan, Y.-C.; Jin, B.-Y.\* On the structural rules of helically coiled carbon nanotubes, *J. Mol. Struct.* **2012** 1008, 1-7.
15. Jin, B.-Y.\* Equation of States for Elections **2012**, *arXiv:1211.1825*.

16. Chuang, C.; Fan, Y.-C.; Jin, B.-Y.\* Systematics of Toroidal, Helically-Coiled Carbon Nanotubes, High-Genus Fullerenes, and Other Exotic Graphitic Materials. *Procedia Engineering*, **2011**, 14, 2373-2385.
17. Hsu, L.-Y.; Tsai, T.-W.; Jin, B.-Y.\* Transport through a mixed-valence molecular transistor in the sequential tunneling regime: theoretical insight from the two-site Peierls-Hubbard model *J. Chem. Phys.* **2010**, 133, 144705.
18. Lin, H.-C.; Jin, B.-Y.\* Charge Transfer Interactions in Organic Functional Materials *Materials* **2010**, 3, 4214-4251.
19. Chang, Y.-W.; Jin, B.-Y.\* Effect of Broken Symmetry on the First Hyperpolarizability of a Centrosymmetric Molecule with an application to furan-containing [2,2]cyclophandiene *J. Chin. Chem. Soc.* **2010**, 57, 575-582.
20. Lin, H.-C.; Jin, B.-Y.\* Interchain Interactions in Organic Conjugated Dimers: The Composite-Molecule Approach *J. Phys. Chem. A* **2010**, 114, 2885–2892.
21. Leung, M.-K.\*; Kuo, L.-C.; Huang, W.-T.; Yang, K.-H.; Jin, B.-Y.; Hsu, H.-F., Alternating Oligo[(2,3-O-Isopropylidene-(L)-threitol)]-co-[(E,E)-1,4-bis(styryl)benzene]: The Linear Chirality Transmission Additivity Relationship in Nematic Liquid Crystals *J. Phys. Chem. B* **2010**, 114, 2607-16.
22. Tsai, T.-W.; Huang, Q.-R.; Peng, S.-M.; Jin, B.-Y.\* Smallest Electric Wire based on Extended Metal Atoms Chains *J. Phys. Chem. C* **2010**, 114, 3641–3644.
23. Chuang, C; Jin, B.-Y.\* Classification of Hypothetical Doubly and Triply Periodic Porous Graphitic Structures by Tilings of Neck-Like Units *J. Math. Chem.* **2010**, 47, 1077-1084.
24. Chuang, C; Jin, B.-Y.\* Hypothetical toroidal, cylindrical, helical analogs of C<sub>60</sub> *J. Mol. Graph. Model.* **2009**, 28, 220-225.
25. Chou, C.-C.; Jin, B.-Y.\* Analytical Expressions of the Vibrational Static Second Hyperpolarizability of Polyacetylene *Chem. Phys.* **2009**, 3 62, 71-74.
26. Chuang, C; Fan, Y.-C.; Jin, B.-Y.\* Dual Space Approach to the Classification of Toroidal Carbon Nanotubes *J. Chem. Info. Model.* **2009**, 49, 1679-1686.
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28. Chou, C.-C.; Jin, B.-Y.\* Vibrational Contributions to Nonlinear Optical Polarizabilities: From Two-Level to Two-Band Systems *Theo. Chem. Acc.* **2009**, 122, 313-324.
29. Chuang, C.; Fan, Y.-C.; Jin, B.-Y.\* Generalized Classification of Toroidal and Helical Carbon Nanotubes *J. Chem. Info. Model.* **2009**, 49, 361-368.
30. Hsu, L.-Y.; Jin, B.-Y.\* An Investigation of Quantum Transport by the Free-Electron Network Model: Resonance and Interference Effects *Chem. Phys.* **2009**, 355, 177-182.
31. Yang, H.-C.; Lee, S.-L.; Chen, C.-H.; Yang, H.-C.; Jin, B.-Y.; Luh, T.-Y.\* One-Handed Helical Double Stranded Polybisnorbornenes *Chem. Comm.* **2008**, 6158-6160.
32. Hsu, L.-Y.; Huang, Q.-R.; Jin, B.-Y.\* Charge Transport Through a Single Molecular Wire Based on Linear Multimetal Complexes: A Non-Equilibrium Green's Function Approach *J. Phys. Chem. C* **2008**, 112, 10538-10541.
33. Hsu, L.-Y.; Jin, B.-Y.\* Bandwidth, Intensity, and Lineshape of the Transmission Spectrum in the Single Molecular Junction *Chem. Phys. Lett.* **2008**, 457, 279-283.

34. Lin, H.-C.; Jin, B.-Y.\* Three Dimensional Through-Space/Through-Bond Delocalization in Cyclophane Systems: A Molecule-in-Molecule Approach *J. Phys. Chem. A* **2008**, 112, 2948-2954.

## Mathematical beading and molecular physical models

1. Horibe, Kazunori; Jin, Bih-Yaw; Tsou, Chia-Chin, From Sangaku Problems to Mathematical Beading: A Hands-on Workshop for Designing Molecular Sculptures with Beads, *Proceedings of Bridges: Mathematical Connections in Art, Music, and Science* **2014**, 503-508.
2. Chuang, C.; Jin, B.-Y. Torus knots with polygonal faces, *Proceedings of Bridges: Mathematical Connections in Art, Music, and Science* **2014**, 59-64.
3. 金必耀、左家靜 珠璣科學之串珠萬花環 科學月刊 **2014**, 533(5), 256-261.
4. 金必耀 從碳簇、準晶到 Zometool 的化學世界 科學研習 **2013**, 52(8), 10-15.
5. Chuang, C.\*; Jin, B.-Y. Construction of Sierpiński Superfullerenes with the Aid of Zome Geometry: Application to Beaded Molecules, *Proceedings of Bridges: Mathematical Connections in Art, Music, and Science* **2013**, 487-490.
6. Tsou, C.-C.; Chuang, C.; Jin, B.-Y.\* Mathematical Beading as Molecular Analog Computation: Beaded Sierpiński Buckyball as an Example, *Proceedings of Bridges: Mathematical Connections in Art, Music, and Science* **2013**, 495-498.
7. 金必耀, 左家靜, 珠璣科學—日本寺廟幾何與正十二面體的串珠模型 **2012**, 33(11) 876-878.
8. 金必耀, 左家靜, 珠璣科學—化學鍵與串珠價球模型, 科學月刊 **2012**, 33(9) 714-717.
9. 金必耀, 左家靜, 珠璣科學—螺旋碼與碳八十的七個同分異構物, 科學月刊 **2012**, 33(7), 556-558.
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11. 金必耀, 左家靜, 珠璣科學—串珠碳六十, 科學月刊 **2012**, 33(3), 230-233.
12. 金必耀, 左家靜, 珠璣科學—八字編與正多面體, 科學月刊 **2012**, 33(1), 72-73.
13. Jin, B.-Y. Super buckyball as a molecular sculpture - its structure and the construction method (分子雕塑—超級珠璣碳球的結構與製作), *CHEMISTRY (The Chinese Chemical Society, Taipei)* 化學季刊 **2012**, 70(3), 1-9.
14. Chuang, C.; Jin, B.-Y.; Wei, W.-C.; Tsou, C.-C. Beaded Representation of Canonical P, D, and G Triply Periodic Minimal Surfaces, *Proceedings of Bridges: Mathematical Connections in Art, Music, and Science*, **2012**, 503-506.
15. Chuang, C.; Jin, B.-Y.\*; Tsou, C.-C.; Tang, N. Y.-Wa; Cheung, M. P. S.; Cuccia, L. A. Molecular Modeling of Fullerenes with Beads, *J. Chem. Edu.* **2012**, 89(3), 414-416.
16. Chuang, C.; Jin, B.-Y.\*; Tsou, C.-C. Designing Sculptures Inspired by Symmetric High-Genus Fullerenes with Mathematical Beading. *Proceedings of Bridges: Mathematics, Music, Art, Architecture, Culture*, **2011**, 523-526.

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18. Jin, B.-Y.\*; Chuang, C.; Tsoo, C.-C. Construction of Physical Models for Arbitrary Fullerenes with Beads: Realization of Tangent-Sphere Model *J. Chin. Chem. Soc.* **2010**, 57, 316-324.
19. Jin, B.-Y.\*; Chuang, C.; Tsoo, C.-C. The Wonderful World of Beaded Molecules (串珠分子模型的美妙世界), *CHEMISTRY (The Chinese Chemical Society, Taipei)* 化學季刊 **2008**, 66, 73-92, in chinese.