

PUBLICATION (1975-2009)

BOOK CHAPTERS AND REVIEWS

1. G.M. Bancroft, H.W. Nesbitt, V.P. Zakaznova-Herzog and J.S. Tse, Turning Points in Solid-State, Materials, and Surface Science, Chapter 39, Edited by K.D. M. Harris and P.P Edwards, published by the Royal Society of Chemistry, 2008.
2. J.S. Tse and D.D. Klug, Phonon Spectroscopy and X-ray Scattering using Synchrotron Radiation, *Physics in Canada*, Sep/Oct, 2006
3. J.S. Tse and D.D. Klug, Recent trends for the Design and Optimization of Thermoelectric Materials – A Theoretical Perspective, *CRC Handbook of Thermoelectrics from Macro to Nano*, ed. R.M. Rowe (2005)
4. J.S. Tse and Y. Ma, First Principles studies of Fe in the earth core, *Trends in Chemical Physics*, 12, 35 (2005).
5. J.S. Tse, Computational High Pressure Science, in *High-Pressure Crystallography*, edited. A. Katrusiak and P. McMillan, NATO Science Series II. Mathematics, Physics and Chemistry, Vol. 140, 179, Kluwer Academic Publishers, London (2004).
6. J.S. Tse, *Ab initio* Molecular Dynamics with Density Functional Theory, *Ann. Rev. Phys. Chem.*, 54, 249 2002.
7. J.S. Tse and D. D. Klug. Molecular dynamics studies of high pressure transformation and structures. R. Winter and J. J. Jonas. Netherlands:Kluwer Academic. *High Pressure Molecular Science* , 1999.
8. J.S. Tse and Z.Q. Li, High performance thermoelectric materials with clathrate structures, *Research Trends in Chem. Phys.*, 9, 91, 2002.
9. J.S. Tse, K. Uehara, Z.Q. Li, R. Rousseau and D.D. Klug, Computer Modeling of the Structures, Stabilities, and Thermoelectric Efficiency of Materials with Clathrate Structures, *Key Engineering Materials*, special edition, Modeling of Materials and its Applications in Advanced Technologies, 227, 136 2002
10. D.D. Klug, J.S. Tse, V. Shpakov, C.A. Tulk, I. Swainson, E.C. Svensson and C.-K. Loong, Transformations, *Dynamics and Structures of Amorphous ices, New Kinds of Phase Transitions* , *Transformation in Disorderd Substances*, V.V Brazhkin, et.al. eds. Kluwer Academic Press, Netherlands 2002
11. J.S. Tse, Recent Advances in Synchrotron Powder Diffraction, in *Chemical Application of Synchrotron Radiation*, edited T.K. Sham, World Scientific, Singapore 2002.

12. **J.S. Tse**, *Powder and Single Crystal Diffraction with Synchrotron radiation*, in Canadian Mineralogy Association of Canada, Monograph, vol.23, edited G. Henderson and D.R. Baker, 43, 2002.
13. D.D. Klug, **J.S. Tse**, E.C. Svensson, I.P. Swainson and C-K. Leong, The Structure and Dynamics of Amorphous and Crystalline phases of Ices. *Science and Technology of High Pressure* (ed. M.H. Manghnani, W.J. Nellis, M.F. Nicol), University Press, p.118, 2000.
14. **J.S. Tse** and R. Rousseau, Ab Initio Molecular Dynamics, *Computational Molecular Spectroscopy*, Ed. P. Jensen and P.R. Bunker, p.625, John Wiley & Sons Ltd, 2000.
15. D.D. Klug, **J.S. Tse**, E.C. Svensson, I.P. Swainson and C-K. Leong, The Structure and Dynamics of Amorphous and Crystalline phases of Ices. *Science and Technology of High Pressure* (ed. M.H. Manghnani, W.J. Nellis, M.F. Nicol), University Press, p.118, 2000.
16. D. D. Klug and **J.S. Tse**. High pressure method. In: *Comprehensive Supramolecular Chemistry*, edited by J.-M. Lehn, United Kingdom:Pergamon, 1996, p. 307.
17. **J.S. Tse**. Molecular modelling and related techniques. In: *Comprehensive Supramolecular Chemistry*, edited by J.-M. Lehn, United Kingdom:Pergamon, 1996, p. 593.
18. G. M. Bancroft and **J.S. Tse**. Ligand field splittings on core levels of main group compounds and metal surfaces from photoelectron spectroscopy. *Comment Inorg. Chem.* 5:89, 1986.

PAPERS CHOSEN TO PUBLISH IN VIRTUAL JOURNAL OF SCIENCE AND TECHNOLOGY

1. Crystal, spin, and electronic structure of the superconductor LiFeAs
Zhi Li, J. S. Tse, and C. Q. Jin
Phys. Rev. B 80, 092503 (2009)
2. Effect of pressure on the iron arsenide superconductor Li_xFeAs ($x=0.8,1.0,1.1$)
S. J. Zhang *et al.*
Phys. Rev. B 80, 014506 (2009)
3. Mechanisms for the formation of H_2 and O_2 from x-ray irradiated dense ice
Yunfeng Liang and John S. Tse
Phys. Rev. B 79, 104105 (2009)
4. X-Ray Raman Spectroscopic Study of Water in the Condensed Phases
John S. Tse, Dawn M. Shaw, Dennis D. Klug, Serguei Patchkovskii, György Vankó,
Giulio Monaco, and Michael Krisch
Phys. Rev. Lett. 100, 095502 (2008)
5. First-principles investigation on the geometry and electronic structure of the three-dimensional cuboidal C_{60} polymer
Jianjun Yang, John S. Tse, and Toshiaki Iitaka
J. Chem. Phys. 127, 134906 (2007)
6. Giant dipole resonance of Ba in $\text{Ba}_8\text{Si}_{46}$: An approach for studying high-pressure induced phase transitions of nanostructured materials
H. Sternemann, C. Sternemann, J. S. Tse, S. Desgreniers, Y. Q. Cai, G. Vankó, N. Hiraoka,
A. Schacht, J. A. Soininen, and M. Tolan
Phys. Rev. B 75, 245102 (2007)
7. Hardness of nanocrystalline diamonds
John S. Tse, Dennis D. Klug, and Faming Gao
Phys. Rev. B 73, 140102 (2006)
8. Graphene nanostructures as tunable storage media for molecular hydrogen
Serguei Patchkovskii, John S. Tse, Sergei N. Yurchenko, Lyuben Zhechkov, Thomas Heine,
and Gotthard Seifert
Proc. Natl. Acad. Sci. U.S.A. 102, 10439 (2005)
9. Ordering of Hydrogen Bonds in High-Pressure Low-Temperature H_2O
Y. Q. Cai *et al.*
Phys. Rev. Lett. 94, 025502 (2005)
10. Electron-phonon coupling in high-pressure Nb
J.S. Tse, Z. Li, K. Uehara, Y. Ma, and R. Ahuja
Phys. Rev. B 69, 132101 (2004)
11. Thermodynamic stability of hydrogen clathrates
Serguei Patchkovskii and John S. Tse
Proc. Natl. Acad. Sci. U.S.A. 100, 14645 (2003)
12. Spontaneous Assembly of Perfectly Ordered Identical-Size Nanocluster Arrays
Jian-Long Li, Jin-Feng Jia, Xue-Jin Liang, Xi Liu, Jun-Zhong Wang, Qi-Kun Xue,
Zhi-Qiang Li, John S. Tse, Zhenyu Zhang, and S. B. Zhang
Phys. Rev. Lett. 88, 066101 (2002)
13. The isotope effect and orientational potentials of methane molecules in gas hydrates
Christian Gutt, Werner Press, Alfred Hüller, John S. Tse, and Helene Casalta

FULL LIST OF PUBLICATIONS

1. N.J. English, **J.S. Tse** and C. Declan, Mechanisms for thermal conduction in various polymorphs of methane hydrate, *Phys. Rev. B*, in press.
2. Y. Yao, **J.S. Tse**, and D.D. Klug, Crystal and electronic structure of superhard BC₅ : First-principles structural optimizations, *Phys. Rev. B*, 80, 094106, 2009.
3. Z. Li, **J.S. Tse**, and C.Q. Jin, Crystal, spin, and electronic structure of the superconductor LiFeAs, *Phys. Rev. B*, 80, 092503, 2009.
4. **J.S. Tse**, Z. Song, Y. Yao, J.S. Smith, S. Desgreniers and D.D. Klug, Structure and electronic properties of BaH₂ at high pressure, *Solid State Comm.*, in press
5. A.A. Leitch, X. Yu, C.M. Robertson, R.A. Secco, **J.S. Tse** and R.T. Oakley, Isostructural Bis-1,2,3-Thiaselenazoly Dimers, *Inorg. Chem.*, (Web): September 18, 2009
6. G.M. Bancroft, H.W. Nesbitt, R. Ho, D.M. Shaw, **J.S. Tse** and M.C. Biesinger, Toward a comprehensive understanding of solid-state core-level XPS linewidths: Experimental and theoretical studies on the Si 2p and O 1s linewidths in silicates, *Phys. Rev. B*, 80, 075405, 2009.
7. Z. Song, J. Yang, and **J.S. Tse**, A Comparative Study on the LDA+U and Hybrid Functional Methods on the Description of the Electronic Structure of YTiO₃ under High Pressure, *Can. J. Chem.*, in press (invited paper dedicated to Prof. T. Ziegler).
8. N.J. English and **J.S. Tse**, Mechanisms for thermal conduction in methane hydrate, *Phys. Rev. Lett.*, 103, 015901 2009
9. **J.S. Tse**, D.D. Klug, S. Desgreniers, J. Smith, R. Dutrisac, Instability of CaLi₂ at High Pressure: Theoretical Prediction and Experimental Results, *Europhys. Lett.*, 86, 56001, 2009
10. S.J. Zhang, X.C. Wang, R. Sammynaiken, **J.S. Tse**, L.X. Yang, Z. Li, Q.Q. Liu, S. Desgreniers, Y. Yao, H.Z. Liu and C.Q. Jin, The effect of pressure on "111" type iron arsenide superconductor Li_xFeAs (x=0.8,1.0,1.1), *Phys. Rev. B*, 80, 014506, 2009.
11. Y. Yao, **J.S. Tse**, J. Sun, D.D. Klug, R. Martoňák and T. Iitaka, Comment on "New Metallic Carbon Crystal", *Phys. Rev. Lett.*, 102, 229601, 2009
12. **J.S. Tse**, Boron charged under Pressure, *Nature*, 457, 800, 2009.
13. J.S. Smith, S. Desgreniers, D.D. Klug and **J.S. Tse**, Strontium hydride remains an insulator up to 113 GPa, *Solid. Stat. Comm.*, 179, 830, 2009.
14. Y. Liang and **J.S. Tse**, Mechanisms for the formation of H₂ and O₂ from x-ray irradiated dense ice, *Phys. Rev. B*, 79, 104105, 2009
15. Y. Xu, **J.S. Tse**, A.R. Oganov, T. Cui, H. Wang and G. Zou, Superconducting high-pressure phase of cesium iodide, *Phys. Rev. B*, 79, 144110, 2009.
16. Y. Yao, **J.S. Tse**, and D.D. Klug, Structures of insulating phases of dense lithium, *Phys. Rev. Lett.*, 102, 115503, 2009.
17. Y. Yao, **J. S. Tse**, Z. Song, D. D. Klug, Core effects on the energetic of solid Li at high pressure, *Phys. Rev. B*, 79, 092103, 2009.
18. J.S. Smith, S. Desgreniers, **J.S. Tse**, J. Sun, D.D. Klug and Y. Ohishi, High-pressure structures and vibrational spectra of barium fluoride: Results obtained under nearly hydrostatic conditions, *Phys. Rev. B*, 79, 134104, 2009.
19. Y. Yao, **J.S. Tse**, K. Tanaka, F. Marsiglio, and Y. Ma, Superconductivity in Lithium, *Phys. Rev. B*, 79, 054524, 2009
20. D. Courmier, D.M. Shaw, S. Patchkovskii and **J.S. Tse**, "A computational study on the X-ray absorption spectrum of proton-ordered crystalline Ice IX, *J. Elect. Spectro. Related Phenom.*, (invited paper), in press.
21. R. Flacau, S. Desgreniers and **J.S. Tse**, Electron Density Topology of Cubic Structure I Xe Clathrate Hydrate at High Pressure, *J. Chem. Phys.*, 129, 244507, 2008.

22. M.Y. Ge, Y.Z. Fang, W. Chen, X. Ye, E.Z. Liu, N.H. Su, K. Stahl, Y.P. Feng, **J.S. Tse**, T. Kikegawa, S. Nakano, Z.L. Zhang, U. Kaiser, F.M. Wu, H.-K. Mao, and J.Z. Jiang: Anomalous compressive behavior in CeO₂ nanocubes under high pressure, *New J. Phys.*, 10, 123016, 2008.
23. Y. He, P. Sharma, K. Biswas, E.Z. Liu, N. Ohtsu, A. Inoue, Y. Inada, M. Nomura, **J.S. Tse**, S. Yin and J.Z. Jiang, Origin of ferromagnetism in ZnO codoped with Ga and Co: Experiment and theory, *Phys. Rev. B* 78, 155202, 2008
24. **J.S. Tse**, Y. Yao, D. D. Klug and S. Desgreniers, Bonding in the ϵ -phase of high pressure oxygen, *J. Phys.: Conf. Ser.* 121 012006 2008
25. Y. Yao, **J.S. Tse**, Z. Song, D.D. Klug, F. Sun and Y. LePage, Structures and Superconducting properties of the High pressure IV and V phases of Ca, *Phys. Rev. B*, 78, 054506, 2008
26. **J.S. Tse** and W. Holzapfel, Equation of state for diamond in wide ranges of pressure and temperature, *J. Appl. Phys.*, . 104 043525, 2008.
27. Y. Meng, P. Eng, **J.S. Tse**, D.M. Shaw, M. Hu, J. Shu, S. Gramsch, C.C. Kao, R.J. Hemley, H-k. Mao, Inelastic x-ray scattering of dense solid oxygen: evidence for intermolecular bonding, *Proc. Natl., Acad. Sci.*, 105, 11640 2008.
28. **J.S. Tse**, D.D. Klug, Y. Yao, and S. Desgreniers, Electronic structure of ϵ -oxygen at high pressure: GW calculations, *Phys. Rev. B* 78, 132101, 2008
29. H. Shimizu, N. Wada, T. Kume , Y. Yao and **J.S. Tse**, Pressure-induced structural transformation in solid xenon studied by Raman spectroscopy, *Phys. Rev. B*, 77, 512101, 2008.
30. Yu. A. Freiman, A.F. Goncharov, S. M. Tretyak, A. Grechnev, **J.S. Tse**, D. Errandonea, H-k. Mao, and R.J. Hemley, Raman scattering in hcp rare gas solids under pressure, *Phys. Rev. B* 78, 014301 2008
31. C. Sternemann, H. Sternemann, S. Huotari, F. Lehmkuhler, M. Tolan and **J.S. Tse**, The barium giant dipole resonance in barite: A study of soft x-ray absorption edges using hard x rays, *J. Anal. At. Spectrom.*, 23, 807 2008 (Hot articles)
32. **J.S. Tse**, D.M. Shaw, D.D. Klug, S.Patchkovskii, G. Vanko, M. Krisch, X-ray Raman spectroscopic study of water in the condensed phases, *Phys. Rev. Lett.*, 100, 095502 2008.
33. M. Eremets, I.A. Trojan, S.A. Medvedev, **J.S. Tse** and Y. Yao, Superconductivity in Hydrogen Dominant Materials: Silane, *Science*, 319, 1506 2008.
34. I. Goncharenko, M.I. Eremets, M. Hanfland, **J.S. Tse** , M. Amboage, Y. Yao and I.A.Trojan, Pressure-induced hydrogen-dominant metallic state in aluminum hydride, *Phys. Rev. Lett.*, 100, 45504, 2008
35. Y. Yao, **J.S. Tse** and K. Tanaka, New metastable high-pressure single-bonded phases of nitrogen from genetic algorithm, *Phys. Rev. B*, 77, 52103 2008.
36. G.M. Bancroft, H.W. Nesbitt, V.P. Zakaznova-Herzog and **J.S. Tse**, Recent Advances in XPS of Non-conductors, *Turning Points in Solid-State, Materials, and Surface Science*, Chapter 39, Edited by K.D. M. Harris and P.P Edwards, published by the Royal Society of Chemistry, 2008.
37. V.P. Zakaznova-Herzog, H.W. Nesbitt, G.M. Bancroft and **J.S. Tse**, Characterization of Leached Layers on Olivine and Pyroxenes using High Resolution XPS and Density Functional Calculations, *Geochimica et Cosmochimica Acta*, 72, 69, 2008
38. **J.S. Tse**, D.D. Klug, Y. Yao, Y. LePage and J.R. Rodgers, Structure and spectroscopic properties of dense solid hydrogen at 160 GPa, *Solid State Comm.*, 145, 5, 2008.
39. M. Volmer, C. Sternemann, **J.S. Tse**, T. Buslaps, N. Hiraoka ,M. Paulus, C. Bull and P.F. McMillan, Charge transfer in silicon clathrates studied by Compton scattering, *Phys. Rev B*, 76, 233104 2007.
40. F. Gao, D.D. Klug and **J.S. Tse**, Theoretical study of new Superhard Materials: B₄C₃, *J. Appl. Phys.*, 102, 084311 2007.
41. J.J. Yang, **J.S. Tse** and T. Iitaka, First-principles investigation on the geometry and electronic structure of the tree-dimensional cuboidal C₆₀ polymer, *J. Chem. Phys.*, 127, 134906, 2007.
42. **J.S. Tse**, R. Flacau, S. Desgreniers and J.Z. Jiang, Electron density topology of high-pressure Ba₈Si₄₆ from a Rietveld and maximum-entropy analysis, *Phys. Rev. B*, 76, 174109, 2007.

43. D.M. Shaw, M. Odelius, **J.S. Tse**, Utility of High Performance Computing Facilities for the Calculation of the Theoretical X-ray Absorption Spectra of Solids, *21st International Symposium on High Performance Computing Systems and Applications*, 4-4, May, 2007, IEEE Computer Society.
44. D.M. Shaw, M. Odelius and **J.S. Tse**, Theoretical X-ray absorption investigation of the uniaxial compression of hexagonal graphite, *Can. J. Chem.*, **85**, 837, 2007.
45. D.M. Shaw and **J.S. Tse**, Theoretical X-ray absorption investigation of high pressure ice and compressed graphite, *J. Phys. Cond. Mat.*, **19**, 425211, 2007.
46. **J.S. Tse**, Y. Yao and Y. Ma, Superconductivity in high pressure solids, *J. Phys. Cond Mat.*, **19**, 425208, 2007.
47. **J.S. Tse**, Y. Song and Z. Liu, Effects of Temperature and Pressure on ZDDP, *Tribiol. Lett.*, **28**, 45 2007.
48. J.S. Smith, S. Desgreniers, **J.S. Tse** and D.D. Klug, High-pressure phase transition observed in barium hydride, *J. Appl. Phys.* **102**, 043520, 2007
49. **J.S. Tse** and D. Shaw, Vibrational dynamics in H⁺-substituted forsterite: A First Principles Molecular Dynamics, *Am. Mineral.*, **92**, 1593, 2007.
50. J.J. Yang, **J.S. Tse**, Y. Yao and T. Iitaka, Structural and Electronic Properties of Pristine and Ba-doped Clathrate-like Carbon Fullerenes, *Angewandte Chemie*, **46**, 6275, 2007.
51. Y. Yao, **J.S. Tse**, Y. Ma and K. Tanaka, Superconductivity in high-pressure SiH₄, *Europhys. Lett.*, **78**, 37003, 2007
52. H. Sternemann, C. Sternemann, **J.S. Tse**, S. Desgreniers, Y. Q. Cai. G. Vanko, N. Hiraoka, A. Schacht, J. A. Soininen and M. Tolan, Giant dipole resonance of Ba in Ba₈Si₄₆: An approach for studying high-pressure induced phase transitions of nanostructured materials, *Phys. Rev. B*, **75**, 245102, 2007
53. Y. Ma and **J.S. Tse**, Ab initio determination of crystal lattice constants and thermal expansion for Germanium Isotopes *Solid State Comm.*, **143**, 161, 2007
54. **J. S. Tse**, D. D. Klug, S. Desgreniers, J. S. Smith, R. Flacau, Z. Liu, J. Hu, N. Chen, and D. T. Jiang, Structural phase transition in CaH₂ at high pressures, *Phys. Rev. B* **75**, 134108 2007
55. **J.S. Tse**, Y. Yao and K. Tanaka, Novel superconductivity in metallic SnH₄ under high pressure, *Phys. Rev. Lett.*, **98**, 117004 2007
56. Y. Xie, **J.S. Tse**, T. Cui, A.R. Oganov, Z. He, Y. Ma, and G. Zou, Electronic and phonon instabilities in face-centered-cubic alkali metals under pressure studied using *ab initio* calculations. *Phys. Rev. B* **75**, 064102 2007
57. Y. Yao and **J.S. Tse**, Electron Phonon Coupling in the High Pressure hcp phase of Xe: A First Principles Study, *Phys. Rev. B*, **75**, 134104 2007
58. I. Lévesque P-O. Bertrand, N. Blouin, M. Leclerc, S. Zecchin, G. Zotti, C.I. Ratcliffe, D.D. Klug, X. Gao, F. Gao and **J.S. Tse**, Synthesis and thermoelectric properties of polycarbazole, polyindolocarbazole and polydiindolocarbazole derivatives, *Chem. Mat.*, **19**, 2128 2007
59. L. Yang, Y. M. Ma, T. Iitaka, **J. S. Tse**, K. Stahl, Y. Ohishi, Y. Wang, R. W. Zhang, J. F. Liu, H.-K. Mao, and J. Z. Jiang, Pressure-induced phase transformations in the Ba₈Si₄₆ clathrate *Phys. Rev. B* **74**, 245209, 2006
60. **J.S. Tse** and D.D. Klug, Phonon Spectroscopy and X-ray Scattering using Synchrotron Radiation, *Physics in Canada*, Sep/Oct, 2006
61. D.D. Klug, **J.S. Tse**, Z. Liu and R.J. Hemley, Hydrogen-bond dynamics and Fermi resonance in high-pressure methane filled ice, *J. Chem. Phys.*, **125**, 154509, 2006
62. H. Liu, **J.S. Tse** and H-k. Mao, Stability of rocksalt phase of zinc oxide under strong compression: Synchrotron x-ray diffraction experiments and first-principles calculation studies, *J. Appl. Phys.* **100**, 093509, 2006
63. P. Heines, H-L. Keller, U. Schwarz, M. Ambruster and **J.S. Tse**, High Pressure Phases of Cs₂[PdI₄].I₂, Cs₂[PBrI₄].I₂ and Cs₂[PdCl₄].I₂, *Inorg. Chem.*, **45**, 9818, 2006

64. J.S. Tse, T. Iitaka and K. Parlinski, Vibrational Properties and Superconductivity in $Ba_{24}Si_{100}$, *Europhys. Lett.*, 75, 153 2006.
65. C. Sternemann, S. Huotari, M. Hakala, M. Paulus, M. Volmer, C. Gutt, T. Buslaps, N. Hiraoka, D.D. Klug, K. Hamalainen, M. Tolan and J.S. Tse, Electronic structure of methane hydrate studied by Compton scattering, *Phys. Rev. B* 73, 195104, 2006
66. X. Gao, D.D. Klug and J.S. Tse, Rational design of high efficiency thermoelectric materials with low band gap conductive polymers, *Comp. Mat. Sci.*, 36, 49 2006
67. J.S. Tse, D.D. Klug, S. Patchkovskii and J.K. Dewhurst, Chemical bonding, electron-phonon coupling, and structural transformations in high-pressure phases of Si, *J. Phys. Chem., B* 110, 3721, 2006
68. J.S. Tse, D.D. Klug, and T. Iitaka, Dynamics of elemental lithium at megabar pressures, *Phys. Rev. B* 73, 212301, 2006
69. J.S. Tse, D.D. Klug and F. Gao, Hardness of nanocrystalline diamonds, *Phys. Rev. B*, 73, 140102, 2006
70. V.V. Struzhkin, H-k Mao, J-F. Lin, R.J. Hemley, J.S. Tse, Y. Ma, M.Y. Hu, P. Chow, and C.C. Kao, Valence band x-ray emission spectra of compressed germanium, *Phys. Rev. Lett.* 96, 137402, 2006
71. A.I. Krivchikov, B. Ya. Gorodilov, O. A. Korolyuk, V. G. Manzhelii, O.O. Romantsova, H. Conrad, W. Press, J.S. Tse, and D.D. Klug, Thermal conductivity of Xe clathrate hydrate at low temperatures, *Phys. Rev. B* 73, 064203, 2006
72. V.P. Zakaznova-Herzog, H.W. Nesbitt, G.M. Bancroft and J.S. Tse, High resolution core and valence band XPS spectra of non-conductor pyroxenes, *Surface Science*, 16, 3175, 2006.
73. I. Lévesque, X. Gao, C.I. Ratcliffe, D.D. Klug, J.S. Tse, N. Blouin, J.-F. Morin, M. Leclerc, New Conjugated Polymers Derived from Carbazole as Thermoelectric Materials, *Mater. Res. Soc. Symp. Proc.* 871E, I9.41.1-6 (2005).
74. I. Lévesque, X.Gao, D.D.Klug, J.S.Tse, C.I.Ratcliffe, Highly soluble poly(2,7-carbazolenevinylene) for thermoelectrical applications: from theory to experiment, *Reactive and Functional Polymers*, 65, 23-36 (2005).
75. J.S. Tse and Y. Ma, First principles studies of Fe in the earth core, *Trends in Chemical Physics*, 12, 35, 2005.
76. J.S. Tse, T. Iitaka, T. Kume, H. Shimizu, K. Parlinski, H. Fukuoka and S. Yamanaka, Electronic properties of Ba_8Si_{46} , $Ba_8Ag_nSi_{46-n}$ and $Ba_8Au_nSi_{46-n}$, *Phys. Rev. B*, 72, 155441, 2005
77. V. P. Zakaznova-Herzog, H. W. Nesbitt, G. M. Bancroft, J. S. Tse, X. Gao, and W. Skinner, High-resolution valence-band XPS spectra of the nonconductors quartz and olivine, *Phys. Rev. B* 72, 205113, 2005
78. Y. Ma, T. Cui, L. Zhang, Y. Xie, G. Zou, J.S. Tse, X. Gao, and D.D. Klug, Electronic and crystal structures of osmium under high pressure *Phys. Rev. B* 72, 174103, 2005
79. J. S. Tse, D. D. Klug, J.Y. Zhao, W. Sturhahn, E.E. Alp, J. Baumert, C. Gutt, M.R. Johnson and W. Press, Anharmonic motions of Kr in the clathrate hydrate. *Nature Materials*, 4, 917, 2005
80. J.S. Tse, D.D. Klug, D.T. Jiang, C. Sternemann, M. Volmer, S. Huotari, N. Hiraoka, V. Honkimaki and K. Hamalainen, Compton Scattering of Elemental Silicon at High Pressure, *Appl. Phys. Lett.*, 87, 191905, 2005
81. Y. Ma, J.S. Tse, T. Cui, D.D. Klug, L. Zhang, Y. Xie, Y. Niu, and G. Zou, First-principles study of electron-phonon coupling in hole- and electron-doped diamonds in the virtual crystal approximation *Phys. Rev. B* 72, 014306, 2005
82. X. Gao, K. Uehara, D.D. Klug, S. Patchkovskii, J.S. Tse, and T.M. Tritt, Theoretical studies on the thermopower of semiconductors and low-band-gap crystalline polymers, *Phys. Rev. B* 72, 125202, 2005
83. J. Baumert, C. Gutt, M. Krisch, H. Requardt, M. Muller, J.S. Tse, D.D. Klug and W. Press, Elastic Properties of Methane Hydrate at High Pressure, *Phys. Rev. B*, 72, 054302, 2005.

84. J.S. Tse and D.D. Klug, Recent trends for the Design and Optimization of Thermoelectric Materials – A Theoretical Perspective, *CRC Handbook of Thermoelectrics from Macro to Nano*, ed. R.M. Rowe (2005)
85. K. Chen, L.R. Zhou, J.S. Tse, Electronic character of interdiffusion of metals in nickel, *J. Mat. Sci.*, 40, 2569 2005.
86. R. Rousseau, K. Uehara, D.D. Klug and J.S. Tse, Phase Stability and Broken Symmetry Transition of Elemental Lithium up to 140 GPa, *Chem. Phys. Chem*, 6, 1703, 2005.
87. H. Liu, J.S. Tse, J. Hu, Z. Liu, L. Wang, J. Chen, D.J. Weidner, Y. Meng, D. Hausermann and H-k. Mao, Structural refinement of high-pressure phase of Aluminium Trihydride: *In-situ* high pressure angle dispersive synchrotron x-ray diffraction and theoretical studies, *J. Phys. Chem.*, **109**, 8857 2005
88. J.S. Tse, D.D. Klug, M. Guthrie, C.A. Tulk, C.J. Benmore and J. Urquidi, The nature of the intermediate and high density forms of amorphous ices, *Phys. Rev. B*, **71**, 214107 2005.
89. C. Sternemann, J.A. Soininen, S. Huotari, G. Vanko, M. Volmer, J.S. Tse and M. Tolan, X-ray Raman Scattering at the L-edges of Na, Si and the N-edge of Ba in Ba₈Si₄₆, *Phys. Rev. B*, **72**, 035104 2005.
90. Y.Q. Cai, H-k. Mao, P.C. Chow, J.S. Tse, Y. Ma, S. Patchkovskii, J.F. Shu, V. Struzhkin, R.J. Hemley, H. Ishii, C.C. Chen, C.T. Chen and C.C. Kao, Ordering of hydrogen bonds in high-pressure-low temperature H₂O, *Phys. Rev. Lett.*, 94, 25502 2005
91. S. Patchkovskii, J.S. Tse, S.N. Yurchenko, L. Zhechkov, T. Heine, G. Seifert, Graphene nanostructures as tunable storage media for molecular hydrogen, *Proc. Natl. Acad. Sci.*, 102, 10439 2005
92. J.S. Tse, Crystallography of High Pressure Elemental Solids, *Z. Krist.*, 220, 521 2005
93. J.S. Tse, Y. Ma and H.M. Tutuncu, Superconductivity in simple elemental solids – a computational study of boron-doped diamond and high pressure phases of Li and Si, *J. Phys. Cond. Matter*, 17, S911 2005.
94. K. Chen, L.R. Zhou, J.S. Tse, Electronic character of interdiffusion of metals in nickel, *J. Mat. Sci.*, 40, 2569 (2005).
95. W. Zhang, C.I. Ratcliffe, I.L. Moudrakovski, J. S. Tse, C-Y Mou and J.A. Ripmeester, Characterization of the location and interfacial states of gallium in gallium/MCM-41 composites, *Microscopic Mesoporous Mat.*, 79, 195 (2005)
96. M. Prager, J. Baumert, W. Press, M. Plazanet, J. S. Tse and D. D.Klug, Adsorption sites and rotational tunneling of methyl groups in cubic I methyl fluoride water clathrate, *Phys. Chem. Chem. Phys.*, 7, 1228 (2005)
97. I. Leveque, X. Gao, D.D. Klug, J.S. Tse, C.I Ratcliffe and M. Leclerc, Highly soluble poly(2,7-carbazolenevinylene) for thermoelectrical application: from theory to experiment, *Reactive and Functional Polymers*, 65, 23 (2005).
98. J.S. Tse, Y. Ma and H.M. Tutuncu, Superconductivity in simple elemental solids – a computational study of boron-doped diamond and high pressure phases of Li and Si, *J. Phys. Cond. Matter*, 17, S911 (2005).
99. X. Gao, J.S. Tse, D.D. Klug and T. Tritt, Theoretical investigation of substitution effects on the electronic structure and transport properties of layered cobalt oxides Na_xCoO₂, *IEEE Trans.*, in press.
100. K. Chen, L.R. Zhao, P.C. Patnaik and J.S. Tse, Elastic Properties of Multi-component Nickel Solid Solutions, *Superalloys 2004*, Edited by K.A. Green, T.M. Pollock, H. Harada, *TMS (The Minerals, Metals & Materials Society)*, 2004
101. G.S. Kim, J.S. Tse and D.D. Klug, Effect of external stress on the patterning of nanostructures: a Kinetic Monte-Carlo simulation of Ta deposited in anisotropically compressed Ta(100) surfaces, *Chem. Phys. Lett.*, 400, 64 (2004)
102. C. Campana, M. Muser, J.S. Tse, D. Herzbach and P. Schoffel, Irreversibility of the pressure-induced phase transition of quartz and the relation between three hypothetical post-quartz phases, *Phys. Rev. B*, 70, 224101 (2004).

103. H.M. Tutuncu, J.S. Tse and G.P. Srivastava, First-Principles Study of Phonon Spectrum of BeS and BeSe, *Phonons in Condensed Materials*, Ed., S P Sanyal, R K Singh, Allied Publishers (2004).
104. K. Chen, L.R. Zhao, J.S. Tse and J.R. Rodgers, *Physics Lett., A*, 331, 400 (2004).
105. Y. Ma, J.S. Tse, D.D. Klug and R Ahuja, Electron-phonon coupling in α -Ga Boron, *Phys. Rev., B*, 70, 214107, 2004.
106. D. D. Klug, J.S. Tse, Z. Liu, X. Gonze and R. J. Hemley, The anomalous transformations in ice VIII, *Phys. Rev. B*, 70, 144113 2004.
107. K. Chen, L.R. Zhao and J.S. Tse, Alloying effect on atomic strengthening of binary Ir solid solutions: a first-principles study, *Materials Letters*. 58, 2852, 2004.
108. M. Guthrie, C.A. Tulk, C.J. Benmore, J. Xu, J.L. Yarger, D.D. Klug, J.S. Tse, H-k. Mao and R.J. Hemley, Formation and structure of a dense octahedral glass, *Phys. Rev. Lett.*, 93, 115520, 2004.
109. X. Gao, J.S. Tse and D.D. Klug, Theoretical Investigation of the electronic structure of $\text{Na}_{1+x}\text{CoO}_2$, *J. Phys. Cond. Matter*, 16, 6493 2004.
110. J.S. Tse, Computational High Pressure Science, in *High-Pressure Crystallography*, edited. A. Katrusiak and P. McMillan, NATO Science Series II. Mathematics, Physics and Chemistry, Vol. 140, 179, Kluwer Academic Publishers, London (2004).
111. T. Kume, T. Koda, S. Sasaki, H. Shimizu, and J.S. Tse, High-pressure Raman study of the potassium-doped silicon clathrate K_8Si_{46} , *Phys. Rev. B* 70, 052101 (2004)
112. J. Baumert, C. Gutt, M.R. Johnson, J.S. Tse, D.D. Klug, and W. Press, The structure of methane hydrate under geological conditions: A combined Rietveld and maximum entropy analysis, *J. Chem. Phys.*, 120, 10163, 2004.
113. J.S. Tse, Z. Li, K. Uehara, Y. Ma and R. Ahuja, Electron-phonon coupling in high-pressure Nb, *Phys. Rev. B*, 69, 132101, 2004.
114. G.S. Kim, J.S. Tse, D.D. Klug and P. Wu, Kinetic Monte Carlo Simulation of Ta Deposition on Ta [100] Surface, *J. Mat. Sci.*, 39, 1519, 2004
115. Y. Ma, J.S. Tse, and D. D. Klug, First-principles study of the mechanisms for the pressure-induced phase transitions in zinc-blende CuBr and CuI, *Phys. Rev. B*, 69, 064102, 2004.
116. K. Chen, L.R. Zhao and J.S. Tse, A first principles survey of γ/γ' interface strengthening by alloying elements in single crystal Ni-based superalloys, *Mat. Sci Eng., A*, 365, 80 2004.
117. J. Baumert, C. Gutt, V.P. Shapkov, J.S. Tse, M. Krisch, M. Muller, H. Requardt, D.D. Klug, S. Jansen and W. Press, Lattice dynamics of methane and xenon hydrate, Observation of symmetry-avoided crossing by experiment and theory, *Phys. Rev. B*, 68, 174301 2003
118. K. Chen, L.R. Zhao, J. Rodgers and J.S. Tse, Alloying effects on elastic properties of TiN-based nitrides, *J. Phys. D*, 36, 2725 2003
119. K. Chen, L.R. Zhao and J.S. Tse, Sulfur embrittlement on γ/γ' interface of Ni-base single crystal superalloys, *Acta Materialia*. 51, 1079 2003
120. K. Chen, L. R. Zhao and J.S. Tse, Synergetic effect of Re and Ru on γ/γ' interface strengthening of Ni-base single crystal superalloys, *Mat. Sci. Eng. A*, 360, 197 2003
121. S. Patchkovskii and J.S. Tse, Thermodynamic Stability of Hydrogen Clathrates, *Proc. Nat. Acad. Sci.*, 100, 14645, 2003.
122. J. Haines, C. Chateau, J.M. Leger, C. Bogicevic, S. Hull, D.D. Klug and J.S. Tse, *Phys. Rev. Lett.*, 91, 015503, 2003.
123. Y. Ma, J.S. Tse and D.D. Klug, Pressure-induced phonon instabilities in copper chloride, *Phys. Rev. B*, 67, 140301R, 2003.
124. H.M. Tutuncu, G.P. Srivastava and J.S. Tse, Structural and dynamical properties of As overlayers on the GaAs(110) surface, *Surf. Sci.* 532, 916, 2003.
125. K. Chen, L.R. Zhao and J.S. Tse, Application of bond order in solid solution strengthening of nickel, *J. Mat. Sci. Lett.*, 22, 603, 2003.
126. K. Chen, L.R. Zhao and J.S. Tse, *Ab initio* study of elastic properties of Ir and Ir_3X compounds, *J. Appl. Phys.*, 93, 2414, 2003.

127. K. Chen, L.R. Zhao, and J.S. Tse, Alloying effects on sulphur embrittlement of the γ - γ' interface of nickel-based single-crystal superalloys, *Phil. Mag. Lett.*, 83, 177, 2003
128. J.S. Loveday, R.J. Nemes, D.D. Klug, J.S. Tse and D.D. Klug, Structural Systematic in the Clathrate Hydrate under Pressure, *Can. J. Phys.*, 81, 539, 2003.
129. J.S. Tse and D.D. Klug, Formation and Decomposition Mechanisms for Clathrate Hydrates, *J. Supramol. Chem.*, 2, 467 2002.
130. H. Nakayama, H. Omi, T. Eguchi, D.D. Klug, J.S. Tse, C.I. Ratcliffe and J.A. Ripmeester, Formation of Gas Hydrate under Curious Conditions as Probe by ^{129}Xe NMR, *The Review of High Pressure Science and Technology*, 12, 10 2002.
131. J.S. Tse, Vibrations of Methane in Structure I Clathrate Hydrate – an *ab initio* Density Functional Molecular Dynamics Study, *J. Supramol. Chem.*, 2, 429 2002.
132. H. Tutuncu, G.P. Srivastava and J.S. Tse, A study of structural, electronic and dynamical properties of Si [011] capped with a monolayer of GaAs, *Phys. Rev. B*, 66, 195305, 2002
133. J.S. Tse, S. Desgrenier, Z.Q. Li, M.R. Ferguson and Y. Kawazoe, Structural Stability and Phase Transitions in K_8Si_{46} Clathrate under High Pressure, *Phys. Rev. Lett.*, 89, 195507, 2002
134. K. Chen, L.R. Zhao and J.S. Tse, Electronic mechanism of γ/γ' interface strength of Ir-based alloys, *J. Phys., Cond. Mat.*, 14, 10041, 2002.
135. M. Geshi, D.D. Klug and J.S. Tse, First-principles studies of pressure-induced phase transitions in SiO_2 , *J. Phys., Condens. Matter* 14, 10891, 2002.
136. D.D. Klug, M. Zgierski, J.S. Tse, Z. Liu, J.R. Kincaid, K. Czarnecki, R.J. Hemley, Dimeric Modes and Dynamics of Model Heme Compounds *Proc. Nat. Acad. Sci.*, 99, 12526, 2002.
137. E.P. van Kaveren, J.J. Michels, J.S. Schouten, D.D. Klug and J.S. Tse, Computer simulation of the dynamics of doubly occupied N_2 clathrate hydrates, *J. Chem. Phys.*, 117, 6637 2002.
138. C. Gutt, W. Press, A. Huller and J.S. Tse, Rotational Dynamics in Methane Hydrates, *Appl. Phys. A*, 74, S1299 2002.
139. C.K. Siu, Z.F. Liu and J.S. Tse, *Ab initio* studies on $\text{Al}^+\text{H}_2\text{O}_n$, $\text{HAIOH}^+\text{H}_2\text{O}_{n-1}$, and the size dependent H_2 elimination reaction, *J. Amer. Chem. Soc.*, 124, 10846, 2002.
140. J.S. Tse, D. D. Klug, V. Shpakov and J. R. Rodgers, High pressure elastic properties of solid argon from first-principles density functional and quasi-harmonic lattice dynamic calculations, *Solid State Comm.* 122, 557, 2002.
141. J.S. Tse, *Ab initio* Molecular Dynamics with Density Functional Theory, *Ann. Rev. Phys. Chem.*, 54, 249 2002.
142. V. P. Shpakov, P. M. Rodger, J.S. Tse, D. D. Klug, and V. R. Belosludov, Thermodynamic discontinuity between low-density amorphous ice and supercooled water, *Phys. Rev. Lett.*, 88, 155502 2002.
143. H.M. Tutuncu, R. Miotto, G.P. Srivastava and J.S. Tse, First principles study of structural and dynamical properties of As overlayers on $\text{InP}[110]$, *Surf. Sci.*, 512, 67 2002.
144. H.M. Tutuncu, R. Miotto, G.P. Srivastava and J.S. Tse, Phonons in $\text{Ga}[110]$, *Appl. Phys. Lett.*, 80, 3322 2002.
145. D.D. Klug, J.S. Tse, V. Shpakov, C.A. Tulk, I. Swainson, E.C. Svensson and C-K. Loong, in *New kinds of Phase Transitions – Transformations in Disordered Substances*, edited by H.E. Stanley and V.V. Brazhkin 2002
146. J. Li, J. Jia, J. Xue, L. Xi, X. Liu, J. Wang, Q. Xue, Z.Q. Li, J.S. Tse, Z. Zhang, and S. B. Zhang, Spontaneous assembly of perfectly ordered identical-size nanocluster arrays, *Phys. Rev. Lett.*, 88, 066101 2002.
147. A. Moewes, E.Z. Kurmaev, J.S. Tse, M. Geshi, M.J. Ferguson, V.A. Trofimova and Y.M. Yarmoshenko, *Phys. Rev. B*, 65, 153106 2002
148. H. Tutunucu, G.P. Srivastava and J.S. Tse, Phonons of group -III nitride 110 surfaces, *Phys. Rev. B*, 66, 115304 2002
149. A. Ker, E. Todorov, R. Rousseau, K. Uehara, F-X. Lannuzel and J.S. Tse, Structure and Phase Stability of Binary Zintl-Phase Compounds, Lithium-Group 13 Intermetallics and Metal-doped Group-14 Clathrate Compounds, *Chem. Eur. J.*, 8, 2787, 2002.

150. J.S. Tse, *Ab initio* Molecular Dynamics with Density Functional Theory, *Ann. Rev. Phys. Chem.*, 54, 249 2002.
151. J.S. Tse and Z.Q. Li, High performance thermoelectric materials with clathrate structures, *Research Trends in Chem. Phys.*, 9, 91, 2002.
152. J.S. Tse, K. Uehara, Z.Q. Li, R. Rousseau and D.D. Klug, Computer Modeling of the Structures, Stabilities, and Thermoelectric Efficiency of Materials with Clathrate Structures, *Key Engineering Materials*, special edition, Modeling of Materials and its Applications in Advanced Technologies, 227, 136 2002
153. D.D. Klug, J.S. Tse, V. Shpakov, C.A. Tulk, I. Swainson, E.C. Svensson and C.-K. Loong, Transformations, *Dynamics and Structures of Amorphous ices, New Kinds of Phase Transitions, Transformation in Disorderd Substances*, V.V Brazhkin, et.al. eds. Kluwer Academic Press, Netherlands 2002
154. J.S. Tse, Recent Advances in Synchrotron Powder Diffraction, in *Chemical Application of Synchrotron Radiation*, edited T.K. Sham, World Scientific, Singapore 2002.
155. J.S. Tse, *Powder and Single Crystal Diffraction with Synchrotron radiation*, in Canadian Mineralogy Association of Canada, Monograph, vol.23, edited G. Henderson and D.R. Baker, 43, 2002.
156. V.I. Belosludov, V.P. Shpako, J.S. Tse, R.V. Belosludov and Y. Kawazoe, Mechanical Stability of Clathrate Hydrates, Chapter 6, *Proceedings of Indo-Russia joint workshop on Gas Hydrates*, Department of Ocean Development, Government of India (2002).
157. J.S. Tse and D.D. Klug, Nucleation, decomposition and guest vibrations in Clathrate Hydrates, *Proceedings of the Fourth International Conference on Gas Hydrates*, p.669, Yokohama, Japan (2002)
158. Z. Li, J.S. Tse and K. Uehara, Phonon Band Structures and Resonant Scattering in $\text{Na}_8\text{Si}_{46}$ and $\text{Cs}_8\text{Sn}_{46}$ Clathrates, *Materials Transactions*, 43, 222, 2002.
160. J. Baumert, C. Gutt, W. Press, J.S. Tse and S. Janssen, Low Frequency Dynamics of Gas Hydrates studied with Inelastic Incoherent Neutron Scattering, *Proceedings of the Fourth International Conference on Gas Hydrates*, p.687, Yokohama, Japan (2002)
161. H. Itoh, J.S. Tse and K. Kawamura, The structure and dynamics of doubly occupied Ar hydrate, *J. Chem. Phys.*, 115:9414, 2001.
162. J. He, D.D. Klug, K. Uehara, K.F. Preston, C.I. Ratcliffe and J.S. Tse, NMR and X-ray Spectroscopy of Sodium-Silicon Clathrates, *J. Phys. Chem.*, B, 105:3475, 2001.
163. J.S. Loveday, R.J. Nelmes, M. Guthrie, S.A. D.D. Klug and J.S. Tse, Transition from Cage Clathrate to Filled Ice: The Structure of Methane Hydrate III., *Phys. Rev. Lett.*, 87:215501, 2001
164. J.S. Loveday, R.J. Nelmes, M. Guthrie, S.A. Belmonte, D.R. Allan, D.D. Klug, J.S. Tse and Y.P. Handa, Existence of stable methane hydrate above 2 GPa and the implication for Titan, *Nature*, 410:661, 2001
165. Z.Q. Li and J.S. Tse, "Reply to comments on Phonon Anomaly in High Pressure Zn", *Phys. Rev. Lett.*, 87:259602, 2001
166. J. Haines, J. M. Leger, F. Gorelli, D.D. Klug, J.S. Tse and Z.Q. Li., X-ray diffraction and theoretical studies of the high-pressure structures and phase transitions in magnesium Fluoride, *Phys. Rev. B* 64:134110 (2001).
167. L. Qui, M.A. White, Z.Q. Li, J.S. Tse, O. Sankey and J.J. Dong, Thermal and Lattice Dynamics of a potential thermoelectric materia : Evidence of enhanced anharmonic interactions in $\text{Na}_8\text{Si}_{46}$, *Phys, Rev. B.*, 64: 024303, 2001
168. Z.Q. Li, K. Uehara and J.S. Tse, Phonon bandstructure and resonant scattering in $\text{Na}_8\text{Si}_{46}$ and $\text{Cs}_8\text{Sn}_{46}$, *Europhys. Lett.*, 56:275, 2001
169. E.P. van Klaveren, J.P.J. Michels, J.A. Schouten, D.D. Klug and J.S. Tse, Molecular Dynamics Simulation study of the properties of doubly occupied N_2 clathrate hydrates, *J. Chem. Phys.*, 115:10500, 2001.
170. J.S. Tse, V.P. Shpakov, V.R. Belosludov, Y.P. Handa, F. Trouw and W. Press, Coupling of Localized Guest Vibrations with the Lattice Modes in Clathrate Hydrates", *Europhys.. Lett.*, 54:354, 2001.

171. D.D. Klug, R. Rousseau, M. Bernasconi, K. Uehara, Y. Le Page and J.S. Tse, *Ab initio* Molecular Dynamics Study of Successive Pressure Induced Transformations in Cristobalite, *Phys. Rev., B*, 63:104106, 2001.
172. C. Gutt, W. Press and J.S. Tse, Isotopic effect and orientational potentials of methane molecules in gas hydrate, *J. Chem. Phys.*, 114:4160, 2001.
173. E.P. van Klaveren, J.P.J. Michels, J.A. Schouten, D.D. Klug and J.S. Tse, Stability of doubly occupied N₂ clathrate hydrates investigated by molecular dynamics simulations, *J. Chem. Phys.*, 114:5745, 2001.
174. I.L. Moudrakovski, S.R. Breeze, B. Simard, C.I. Ratcliffe, J.A. Ripmeester, T. Seideman, J.S. Tse and G. Sanytr, Gas-phase nuclear magnetic relaxation in ¹²⁹Xe revisited. *J. Chem. Phys.*, 114:2173, 2001
175. R.V. Belosludov, V.P. Shpakov, V.R. Belosludov, N.D. Luzhkovskaya, Y. Kawazoe, J. S. Tse, Lattice dynamics simulations of resonant scattering of lattice phonons of clathrate compounds by guest atoms. , in "*Intelligence in a Materials World. Selected papers from IPMM2001*", CRC PRESS (2001) 367-375
176. V.R. Belosludov, T.M. Inerbaev, V.P. Shpakov, J.S. Tse, R.V. Belosludov and Y. Kawazoe, Elastic moduli and stability of ices and clathrate hydrates of cubic structure I. Russian Chemical Journal XLV (3) 45-50. 2001. (in Russian)
177. D.D. Klug, J.S. Tse, E.C. Svensson, I.P. Swainson and C-K. Leong, The Structure and Dynamics of Amorphous and Crystalline phases of Ices. *Science and Technology of High Pressure* (ed. M.H. Manghnani, W.J. Nellis, M.F. Nicol), University Press, p.118, 2000.
178. Z.Q. Li and J.S. Tse, Phonon Anomaly in High Pressure Zn, *Phys. Rev. Lett.*, 85:5130 2000.
179. J.S. Tse, D.D. Klug, C.A. Tulk, E.C. Svensson, I. Swainson, V.P. Shpakov and V.R. Belosludov, Origin of Low-Frequency Local Vibrational Modes in High Density Amorphous Ice, *Phys. Rev. Lett.*, 85:3185, 2000.
180. Berces, O. Koentjoro, B.T. Strenberg, J.H. Yamamoto, J.S. Tse and A.J. Carty, Electronic Structures of Transition Metals Phosphorus Monoxide Compounds, *Organometallics*, 19:4336, 2000.
181. J.S. Tse and R. Rousseau, Ab Initio Molecular Dynamics, *Computational Molecular Spectroscopy*, Ed. P. Jensen and P.R. Bunker, p.625, John Wiley & Sons Ltd, 2000.
182. Z. Li and J.S. Tse, High Pressure bct to fcc structural transformation in Ga, *Phys. Rev., B*, 62:9900 2000.
183. V.R. Belosludov, V.P. Shpakov, J.S. Tse, R.V. Belosludov and Y. Kawazoe, Mechanical stability of Gas Hydrates under Pressure, *Annals New York Academy of Sciences*, 912, 993-1002 2000.
184. B.S. Hudson, J.S. Tse, M.Z. Zgierski, S.F. Parker, D.A. Braden and C. Middleton, The inelastic incoherent neutron spectrum of crystalline oxamide: experiment and simulation of a solid, *Chem. Phys.*, 261:249, 2000.
185. C. Gutt, B. Amussen, W. Press, M.R. Johnson, Y.P. Handa and J.S. Tse, The Structure of Methane Hydrate, *J. Chem. Phys.*, 113:4713, 2000.
186. R. Rousseau and J.S. Tse, Rationalization of Structures of Binary Alloys in a Real Space Atomic Level Perspective, *Prog. Theoret. Phys., Suppl.* 138:47 2000.
187. K. Uehara and J.S. Tse, First Principles Calculation of the Electronic Transport Properties of Metals, *Prog. Theoret. Phys., Suppl.* 138,:113 2000.
188. J.S. Tse, D.D. Klug, K. Uehara, Z.Q. Li, J. Haines and J.M. Leger, Elastic Properties of Potential Superhard Phases of RuO₂, *Phys. Rev. B.*, 61:10029 2000
189. J. Xie, S.P. Chen, J.S. Tse, D.D. Klug, Z.Q. Li, K. Uehara and L.G. Wang, Phonon Instabilities in high-pressure bcc-fcc and the isostructural Phase Transitions of Cs, *Phys. Rev. B*, 62:3624, 2000.
190. J.S. Tse, K. Uehara, R. Rosseau, A. Ker, C.I. Ratcliffe, M.A. White and G. Mackay, Structural Principles and Amorphous-like Thermal Conductivity of Na-doped Si Clathrates, *Phys. Rev. Lett.*, 85:114, 2000.

191. Z.Q. Li and J.S. Tse, Ab initio studies on the vibrational and thermal properties of Al₃Li, *Phys. Rev., B*, 61:14531 2000.
192. Z.F. Liu, W.L. Yim, J.S. Tse and J. Hafner, Ab initio molecular dynamics on Ag_n (n=4,5,6), *Europhy. Phys. J. D*, 10:105 2000.
193. K. Uehara and J.S. Tse, The implementation of the iterative diagonalization scheme and *ab-initio* molecular dynamics simulation in the LAPW method, *Mol. Simul.*, 23:343 2000.
194. K. Uehara and J.S. Tse, Calculations of Transport Properties using Linearized Plane Wave Method, *Phys. Rev., B*, 61:1639 2000.
195. J.S. Tse, V.P. Shpakov and V.R. Belosludov, Vibrational spectrum, elastic moduli and mechanical stability of ice VIII, *J.Chem.Phys.*, 24:11111 1999
196. C. Gutt, B. Asmussen, W. Press, C. Merkl, H. Casalta, J. Greinert, G. Bohrmann, E. Suess, J.S. Tse and A. Huller, Quantum Rotations in Natural Methane-Clathrates from the Pacific Seafloor, *Europhys.Lett.*, 48:269 1999.
197. Z.F. Liu, C.K. Siu and J.S. Tse, Ab initio molecular dynamics study on the hydrolysis of molecular chlorine, *Chem. Phys. Lett.*, 311:93 1999.
198. J. Xie, S.P. Chen, J.S. Tse, S. de Gironcoli and S. Baroni, High Pressure thermal expansion, bulk modulus and phonon structures of diamond, *Phys.Rev.B*, 60:9444, 1999
199. Z. F. Liu, C. K. Siu and J.S. Tse, Catalysis of the reaction HCl + HOCl → H₂O + Cl₂ on an ice surface, *Chem. Phys. Lett.*, 309:335, 1999
200. S. P. Chan, Z. F. Liu, W. M. Lau, and J.S. Tse. SiCl₄ desorption in chlorine etching of Si(100) - a first principle study. *Surf.Sci.* 432:125, 1999.
201. J. He, Y. Ba, C. I. Ratcliffe, J. A. Ripmeester, D. D. Klug, and J.S. Tse. The nature of encapsulated silicon nanoclusters in zeolite Y. *Appl.Phys.Lett.* 74:830, 1999.
202. P. J. Low, R. Rousseau, P. Lam, K. A. Udachin, G. D. Enright, J.S. Tse, D. D. M. Wayner and A.J. Carty. Polycarbon ligand chemistry: electronic interactions between a mononuclear ruthenium fragment and a cobalt-carbon cluster core. *Organometallics*, 18:3885, 1999.
203. J.S. Tse, G. Frapper, A. Ker, R. Rousseau, and D. D. Klug. Phase stability and electronic structure of K-Ag intermetallics at high pressure. *Phys.Rev.Lett.* 82:4472, 1999.
204. J.S. Tse, D. D. Klug, C. A. Tulk, I. P. Swainson, E. C. Svensson, C-K. Loong, V. P. Shpakov, V. R. Belosludov, R. V. Belosludov, and Y. Kawazoe. The mechanisms for pressure-induced amorphization of ice Ih. *Nature* 400:647, 1999.
205. K. Uehara and J.S. Tse, Soft X-ray fluorescence spectra of photoluminescent layered polysilanes, *Chem. Phys. Lett.*, 301:474, 1999.
206. J.S. Tse and D. D. Klug. Molecular dynamics studies of high pressure transformation and structures. R. Winter and J. J. Jonas. Netherlands:Kluwer Academic. *High Pressure Molecular Science*, 1999.
207. J.S. Tse and D. D. Klug. Structure and dynamics of liquid sulphur. *Phys.Rev.B* 59:34, 1999.
208. Courtney, J.S. Tse, O. Mao, J. Hafner, and J. R. Dahn. Ab initio calculation of the Lithium-Tin Voltage Profile. *Phys.Rev.B* 58:15583, 1998.
209. L. L. East, Z. F. Liu, C. McCague, K. Cheng, and J.S. Tse. The three isomer of protonated ethane, C₂H₇⁺. *J.Phys.Chem.A* 102:10903, 1998.
210. J. He, Y. Ba, C. I. Ratcliffe, J. A. Ripmeester, D. D. Klug, J.S. Tse, and K. F. Preston. Encapsulation of silicon nanoclusters in zeolite Y. *J.Am.Chem.Soc.* 120:10697-10705, 1998.
211. J. He, J.S. Tse, D. D. Klug, and K. F. Preston. Layered polysilane: thermolysis and photoluminescence. *J.Mat.Chem.* 8:705, 1998.
212. V. P. Shpakov, J.S. Tse, C. A. Tulk, B. Kvamme, and V. R. Belosludov. Elastic moduli calculation and instability of structure I methane hydrate. *Chem.Phys.Lett.* 282:107, 1998.
213. J.S. Tse, V. P. Shpakov, and R. V. Belosludov. High pressure elastic constants of solid krypton from quasiharmonic lattice dynamics calculations. *Phys.Rev.B* 58:2365, 1998.
214. J.S. Tse and D. D. Klug. The anomalous isostructural transformation in ice VIII. *Phys.Rev.Lett.* 81:2466, 1998.
215. J.S. Tse, G. Frapper, V. I. Smelyansky, and D. D. Klug. Electronic structure and bonding analysis in K-Ag alloys. *Rev.High Press.Sci.Technology* 7:163, 1998.

216. Coulthard, T. K. Sham, J. D. Garret, V. I. Smelyansky, and J.S. Tse. XAFS of early 4d transition metal silicides - 4d metal $L_{2,3}$ and Si K-edge studies. *J.de Phys.IV*7:497, 1997.
217. J. He, D. D. Klug, J.S. Tse, C. I. Ratcliffe, and K. F. Preston. Luminescent intrazeolitic Si nanoclusters: size study by Si K- and $L_{2,3}$ -x-ray absorption near-edge structure, x-ray photoelectron and photoluminescence spectroscopies. *Appl.Phys.Lett.* 71 (22):3194-3196, 1997.
218. J. He, D. D. Klug, J.S. Tse, and K. F. Preston. X-ray absorption and photoelectron spectroscopic observation of intrazeolitic silicon nanoclusters. *Chem.Comm.*:1265-1266, 1997.
219. Y. F. Hu, G. M. Bancroft, H. B. Davis, J. L. Male, R. K. Pomeroy, J.S. Tse, and K. H. Tan. Electronic structure of $Os(Co)_4L$ ($L=CO, PMe_3$) studied by variable-energy photoelectron spectroscopy. *Organometallics* 15:4493, 1997.
220. K. L. Kavanagh, B. Leduc, T. Pinnington, T. Tiedje, D. D. Klug, and J.S. Tse. In situ detection of misfit dislocation by light scattering. *J.Cryst.Growth* 174:550, 1997.
221. H. Nakayama, D. H. Brouwer, Y. P. Handa, D. D. Klug, J.S. Tse, C. I. Ratcliffe, X. Zhu, and J. A. Ripmeester. Methanol: clathrate hydrate former or inhibitor? *Gas Hydrates Symposium Preprints of the Division of Fuel Chemistry of the American Chemical Society* 42(Division of Fuel Chemistry):516-521, 1997..
222. S. J. Natfel, T. K. Sham, V. I. Smelyansky, J.S. Tse, and J. D. Garret. Angular dependent XAFS studies of a $MoSi_2$ single crystal. *J.de Phys.IV*7 (495), 1997.
223. V. P. Skpakov, J.S. Tse, V. R. Belosludov, and R. V. Belosludov. Elastic moduli and instability in molecular crystals. *J.Phys.Condens.Matter* 9:5835, 1997.
224. V. I. Smelyansky and J.S. Tse. The electronic structure of metallo-silicon clathrates. *Chem.Phys.Lett.* 264:459, 1997.
225. J.S. Tse, V. P. Shpakov, V. V. Murashov, and R. V. Belosludov. The low frequency vibrations in clathrate hydrates. *J.Chem.Phys.* 107:9271, 1997.
226. J.S. Tse, D. D. Klug, Y. LePage, and M. Bernasconi. High pressure 4-coordinated structure of SiO_2 . *Phys.Rev.B* 56:19878, 1997.
227. J.S. Tse, C. I. Ratcliffe, B. M. Powell, V. F. Sears, and Y. P. Handa. Rotational and translational motions of trapped methane. Incoherent and inelastic neutron scattering of methane hydrate. *J.Phys.Chem.A* 101:4491-4495, 1997.
228. J.S. Tse. Electronic and vibrational properties of gas hydrates. *Preprints of the Division of Fuel Chemistry of the American Chemical Society* 42:534, 1997.
229. Y. F. Hu, G. M. Bancroft, H. B. Davis, J. L. Male, R. K. Pomeroy, J.S. Tse, and K. H. Tan. Electronic structure of $Os(CO)_4L$ ($L = CO, Prme_3$) studied by variable-energy photoelectron spectroscopy. *Organometallics* 15:4493, 1996.
230. Y. F. Hu, G. M. Bancroft, K. H. Tan, J.S. Tse, and D. S. Yang. Variable-energy photoelectron spectroscopy of $CpM(CO)_3$ ($M = Mn, Re$) and $CpFe(CO)_2$. *Can.J.Chem.* 74:2240, 1996.
231. D. D. Klug and J.S. Tse. High pressure method. In: *Comprehensive Supramolecular Chemistry*, edited by J.-M. Lehn, United Kingdom:Pergamon, 1996, p. 307.
232. Y. LePage, D. D. Klug, and J.S. Tse. Derivation of conventional crystallographic descriptions of new phases from results of *ab initio* inorganic structure modelling. *J.Appl.Cryst.* 29:503, 1996.
233. X. Li, J.S. Tse, G. M. Bancroft, R. J. Puddapatt, and K. H. Tan. Variable energy photoelectron spectroscopy of $(\eta^5-C_5H_5)NiNO$: molecular orbital assignment and $X\alpha$ - SW calculations. *Inorg.Chem.* 35:2515, 1996.
234. V. P. Skpakov, J.S. Tse, V. R. Belosludov, and R. V. Belosludov. Elastic moduli and instability in molecular crystals. *J.Phys.Condens.Matter* 9:5835, 1996.
235. V. I. Smelyansky and J.S. Tse. The electronic structure of metallo-silicon clathrates. *Chem.Phys.Lett.* 264 (459), 1996.
236. J.S. Tse. Molecular modelling and related techniques. In: *Comprehensive Supramolecular Chemistry*, edited by J.-M. Lehn, United Kingdom:Pergamon, 1996, p. 593.
237. J.S. Tse and D. D. Klug. The structure and dynamics of high pressure phases of hydrogen. Singapore:World Scientific. *Proc.of Joint AIRAPT and EHPRG Int'l Conference* :530, 1996. .

238. D. W. Boo, Z. F. Liu, A. G. Suits, **J.S. Tse**, and Y. T. Lee. Dynamics of carbonium ions solvated by molecular hydrogen: $\text{CH}_5^+(\text{H}_2)_n$ ($n=1,2,3$). *Science* 269:57, 1995.
239. J. A. Howard, C. McCague, R. Stuchliffe, **J.S. Tse**, and H. A. Joly. Electron paramagnetic resonance spectroscopy study of the reaction of Al and Ga atoms with CO_2 and CS_2 in a rotating cryostat. *J.Chem.Soc.Faraday Trans.II* 91:799, 1995.
240. M. Kolbuszewski and **J.S. Tse**. On the bonding and structure of ethylene - BrCl adducts. *Chem.Phys.Lett.* 236:189, 1995.
241. X. Li, **J.S. Tse**, G. M. Bancroft, R. J. Puddephatt, and K. H. Tan. Variable-energy photoelectron spectroscopy of $(\eta^5\text{-C}_5\text{H}_5)_M$ of $(\eta^5\text{-C}_3\text{H}_5)$ ($M=\text{Ni}$ and Pd), molecular orbital assignments. *Organometallics* 14:4513, 1995.
242. Z. F. Liu, G. M. Bancroft, **J.S. Tse**, and H. Agren. A MCSCF and local density functional study of the vibrational structures in core level photoelectron spectrum. *Phys.Rev.A* 51:439, 1995.
243. Z. F. Liu, G. M. Bancroft, **J.S. Tse**, and Z. Z. Yang. MSX α studies of the $L_{2,3}$ near edge photoabsorption spectra of XH_n , $X = \text{Si}, \text{P}, \text{S}, \text{Cl}$ and $n = 4, 3, 2, 1$. *Chem.Phys.* 192:255, 1995.
244. V. V. Murashov, L. S. Dubrovinski, **J.S. Tse**, and Y. LePage. Pressure-induced phase transition of α -cristobalite form of GaPO_4 . *J.Phys.Condens.Matter* 7:8279, 1995.
245. V. I. Smelyansky and **J.S. Tse**. Theoretical study of the high-pressure phase transformation in ZnSe. *Phys.Rev.* B52:4658, 1995.
246. **J.S. Tse**, D. D. Klug, and D. C. Allan. The structure and stability of several high pressure polymorphs of silica. *Phys.Rev.B* 51:16392, 1995.
247. **J.S. Tse**, J. R. Dahn, and F. Buda. Electronic structure of layered polysilanes. *J.Phys.Chem.* 89:1896, 1995.
248. **J.S. Tse** and D. D. Klug. Evidence from molecular dynamics simulations for non-metallic behaviour of solid hydrogen at 160 GPa. *Nature* 378:595, 1995.
249. **J.S. Tse** and D. D. Klug. Comments on Li et al. evidence for two kinds of H-bonds in ice. *Phys.Lett.* A198:464, 1995.
250. **J.S. Tse** and D. D. Klug. Theoretical studies of structural stability at high pressure. *J.Phys.* 73:253, 1995.
251. **J.S. Tse** and D. D. Klug. Reversible amorphization and structural memory effect in clathrasil dodecasil-3C. *Supramol.Chem.* 6:163, 1995.
252. **J.S. Tse**, D. D. Klug, and K. Laasonen. Structural dynamics of protonated methane and acetylene. *Phys.Rev.Lett.* 74:876, 1995.
253. S. K. Brownstein, P. Y. Plouffe, P. Y. Bensimon, and **J.S. Tse**. Complexes of Tris (2-pyridyl) amines with lithium and sodium salts. *Inorg.Chem.* 33:354, 1994.
254. R. E. Bursten, J. C. Green, N. Kaltsoyannis, **J.S. Tse**, K. H. Sze, and M. H. McDonald. Variable photon energy photoelectron spectroscopic and theoretical investigations of the electronic structure of TiCl_4 . *Inorg.Chem.* 33:5086, 1994.
255. J. R. Dahn, B. M. Way, E. Fuller, W. J. Weydanz, **J.S. Tse**, D. D. Klug, T. Buren, and T. Tiedje. X-ray diffraction and x-ray absorption studies of porous silicon, siloxene, heat-treated siloxene, and layered polysilane. *J.Appl.Phys.* 75:1946, 1994.
256. H. A. Joly, J. A. Howard, M. Tomietto, and **J.S. Tse**. Characterization of the intermediates formed in the reaction of Al atoms with H_2O , H_2S and H_2Se by EPR spectroscopy. *J.Chem.Soc.Perkin II* 90:3145, 1994.
257. J. A. Ripmeester, C. I. Ratcliffe, D. D. Klug, and **J.S. Tse**. Molecular perspectives on structure and dynamics in clathrate hydrates. *Ann.New York Acad.Sci.* 715:161-176, 1994.
258. **J.S. Tse** and D. D. Klug. Ab initio molecular dynamics study on the thermal stability of Na_8 microcluster. *J.Chem.Phys.* 101:473, 1994.
259. **J.S. Tse**. Dynamical properties of clathrate hydrates. *Ann.New York Acad.Sci.* 715:187, 1994.
260. **J.S. Tse**, D. D. Klug, and Z. Lu. X-ray photoelectron and x-ray photoabsorption study of pressure amorphized T- Nb_2O_5 . *Phys.Rev.B* 49:9180, 1994.

261. J.S. Tse. Localized oscillators and heat conduction in clathrate hydrates. *J.Incl.Phenom.* 17:259, 1994.
262. J.S. Tse, D. D. Klug, J. A. Ripmeester, S. Desgreniers, and K. Lagerec. The role of non-deformable units in pressure-induced reversible amorphization of clathracils. *Nature* 369:724, 1994.
263. J.S. Tse and D. D. Klug. Molecular dynamics studies of high-pressure phase transitions and structures. in: High-Pressure Science and Technology. S. C. Schmidt, J. W. Shaner, G. A. Samara, and M. Ross. New York:American Institute of Physics. *Proc.IRPAT 1993*, 1994.
264. G. M. Bancroft, J. D. Bozek, J. N. Cutler, Y. F. Hu, Z. F. Liu, D. G. Sutherland, K. H. Tan, and J.S. Tse. High resolution core level photoemission of molecules. F. J. Wuilleumier, Y. Petroff, and I. Nenner. New Jersey:World Scientific. *Proc.of Intl.Conference Vacuum Ultraviolet Radiation* (Vacuum Ultraviolet Radiation Physics):191, 1993. .
265. J. R. Dahn, B. M. Way, E. Fuller, and J.S. Tse. Structure of siloxene and layered polysilane (Si_6H_6). *Phys.Rev.* B48:17872, 1993.
266. J.S. Tse, M. A. Desando, J. A. Ripmeester, and Y. P. Handa. Thermally induced phase transformations in clathrasil dodecasil-3C. The role of guest molecules. *J.Am.Chem.Soc.* 115:281, 1993.
267. J.S. Tse, D. D. Klug, and B. X. Yang. The use of soft x-rays of very long wavelengths for small angle scattering at the Aladdin storage ring. *J.Appl.Cryst.* 26:130, 1993.
268. J.S. Tse and D. D. Klug. Pressure-induced order-disorder transformations. *Order/Disorder in solids* 9:1, 1993.
269. J.S. Tse, B. M. Powell, V. F. Sears, and Y. P. Handa. The lattice dynamics of clathrate hydrates. An incoherent inelastic neutron scattering study. *Chem.Phys.Lett.* 215:383, 1993.
270. J.S. Tse and D. D. Klug. Anisotropy in the structure of pressure-induced disordered solids. *Phys.Rev.Lett.* 70:174, 1993.
271. J.S. Tse, D. D. Klug, J. A. Ripmeester, and M. Zakrzewski. The thermal expansion of clathracil Dodecasil-3C. *Zeolites* 13:374, 1993.
272. J. A. Howard, R. Jones, J.S. Tse, M. Tomietto, P. L. Timms, and A. J. Seeley. Matrix isolation EPR study of the reaction of Ag atoms with PN, SiS and GeO. *J.Phys.Chem.* 96:9144, 1992.
273. D. D. Klug, J.S. Tse, and E. Whalley. The role of long-range electrical forces in the infrared spectrum of Ice I_h . In: *Physics and Chemistry of Ice*, edited by N. Maeno and T. Hondoh, Sapporo, Japan:Hokkaido University Press, 1992, p. 88.
274. Z. F. Liu, J. N. Cutler, G. M. Bancroft, K. H. Tan, R. G. Cavell, and J.S. Tse. Crystal field splittings of continuum d orbital. Comparative study of the $L_{2,3}$ edge X-ray absorption spectra of Si, P and S compounds. *Chem.Phys.* 168:133, 1992.
275. Z. F. Liu, G. M. Bancroft, J. N. Cutler, D. G. Sutherland, K. H. Tan, J.S. Tse, and R. G. Cavell. Vibrational structure in core level photoelectron spectra: periodic trends. *Phys.Rev.* A46:1688, 1992.
276. V. F. Sears, B. M. Powell, J.S. Tse, C. I. Ratcliffe, and Y. P. Handa. Motion of CH_4 molecules in D_2O clathrate from incoherent inelastic neutron scattering. *Physica B: Condens.Matter.* 180 & 181:658, 1992.
277. J.S. Tse and D. D. Klug. The mechanisms for pressure-induced amorphization and the reverse crystalline transformation in solids. *EOS Trans.Amer.Geophys.Union.* 73:580, 1992.
278. J.S. Tse, D. D. Klug, and Y. LePage. High pressure densification of amorphous silica. *Phys.Rev.* B46:5933, 1992.
279. J.S. Tse, D. D. Klug, and Y. LePage. A novel high pressure form of silica. *Phys.Rev.Lett.* 69:3647, 1992.
280. J.S. Tse. Mechanical instability in Ice I_h . A mechanism for pressure-induced amorphization. *J.Chem.Phys.* 96:5482, 1992.
281. J.S. Tse. Pressure induced amorphization of ice and clathrate hydrates. In: *Physics and Chemistry of Ice*, edited by N. Maeno and T. Hondoh, Hokkaido University Press, 1992, p. 90.

282. J.S. Tse, D. D. Klug, and Y. LePage. High pressure densification of amorphous silica. *Phys.Rev.B* 46:5933, 1992.
283. J.S. Tse and D. D. Klug. Structural memory in pressure-amorphized ALPO₄. *Science* 255:1559, 1992.
284. J.S. Tse and D. D. Klug. High pressure phase transitions in silica and berlinite by molecular dynamics simulations. In: *Recent Trends in High Pressure Research*, edited by A. K. Singh, New Delhi:Vedams Book International, 1992, p. 274.
285. G. W. Buchanan, V. Morat, R. A. Kirby, and J.S. Tse. The hydroxoium perchlorate complex of cis-syn-cis dicyclohexane 18-crown-6 ether conformational analysis in the solid state and in solution at low temperature as studied via ¹³C NMR methods. *Can.J.Chem.* 69:1964, 1991.
286. Y. P. Handa, J.S. Tse, D. D. Klug, and E. Whalley. Pressure-induced phase transitions in clathrate hydrates. *J.Chem.Phys.* 94:623, 1991.
287. R. C. Hynes, K. F. Preston, J. J. Springs, J.S. Tse, and A. J. Williams. Electron paramagnetic resonance studies of radical pairs [M(CO)₅]⁻₂ (M = Cr, Mo, W) trapped in single crystals of PPh₄⁺HM(CO)₅⁻. *Faraday Trans.J.Chem.Soc.* 87:3121, 1991.
288. D. D. Klug, J.S. Tse, and E. Whalley. The longitudinal optic - transverse optic mode splitting in ice Ih. *J.Chem.Phys.* 95:7071, 1991.
289. J.S. Tse and D. D. Klug. The structure and dynamics of silica polymorphs using a two-body effective potential model. *J.Chem.Phys.* 95:9176, 1991.
290. J.S. Tse, D. D. Klug, D. A. Wilkinson, and Y. P. Handa. Phase transitions in solid C₆₀. *Chem.Phys.Lett.* 183:387, 1991.
291. J.S. Tse and D. D. Klug. Mechanical instability of α-quartz: a molecular dynamics study. *Phys.Rev.Lett.* 67:3559, 1991.
292. J.S. Tse and Z. F. Liu. Characterization of Rydberg transitions in the L_{2,3} absorption spectra of SF₆ and PF₅. *Phys.Rev.* A44:7838, 1991.
293. Y. P. Handa, C. I. Ratcliffe, J.S. Tse, and J. A. Ripmeester. Structural transitions in mixed hydrates of structure I and structure II hydrates formers. *J.Phys.Chem.* 94:4363, 1990.
294. Z. F. Liu, J. N. Cutler, G. M. Bancroft, K. H. Tan, R. G. Cavell, and J.S. Tse. High resolution gas phase photoabsorption spectra and multiple scattering Xα study of PX₃ (X=H,CH₃,CF₃) compounds at the P L_{2,3} edge. *Chem.Phys.Lett.* 172:421, 1990.
295. J.S. Tse. Stability and potential energy surface of the three low lying states of Al₃. *J.Chem.Phys.* 92:2488, 1990.
296. J.S. Tse. Thermal expansion of structure--H clathrate hydrates. *J.Incl.Phenom.* 8:25, 1990.
297. J.S. Tse, K. H. Tan, and J. M. Chen. Oxygen K-edge XANES of crystalline and amorphous ice. *Chem.Phys.Lett.* 174:603, 1990.
298. J.S. Tse. A bridge structure for the Ag...SiO adduct. *J.Chem.Soc.Chem.Commun.:*1179, 1990.
299. J.S. Tse. A MP2 and MCSCF/CI study on the stability of Al-acetylene adducts. *J.Am.Chem.Soc.* 112:5060, 1990.
300. J.S. Tse and M. L. Klein. Pressure induced amorphization of ice I_h. *J.Chem.Phys.* 92:3992, 1990.
301. D. S. Yang, G. M. Bancroft, R. J. Puddephatt, and J.S. Tse. The electronic structure of square-planar cis-bis (trifluoromethyl) platinum(II) complex from UV photoelectron spectra and SCF-MS-Xα calculations. *Inorg.Chem.* 29:2496, 1990.
302. D. S. Yang, G. M. Bancroft, L. Dignard-Bailey, R. J. Puddephatt, and J.S. Tse. The electronic structure of cis -dimethylplatinum(II) complexes from UV photoelectron spectra and SCF-MS-Xα calculations. *Inorg.Chem.* 29:2487, 1990.
303. B. W. Yates, G. A. Wald, J. W. Taylor, J.S. Tse, and F. A. Grimm. Angle-resolved photoelectron study of the group VI B metal hexacarbonyls M(CO)₆ (M=Cr,Mo,W) from 9 to 30 eV photon energy. *Chem.Phys.* 147:431, 1990.
304. B. M. Addison-Jones, K. H. Tan, B. W. Yates, J. N. Cutler, G. M. Bancroft, and J.S. Tse. A comparison of valence level photoelectron cross sections for SF₆, SeF₆ and "F₆" from 21 eV to 100 eV photon energy. *J.Electron.Spectrosc.Relat.Ph.* 48:155, 1989.

305. M. Badaye, R. P. Gupta, and J.S. Tse. A pulsed plasma source for soft X-rays spectroscopy. *Physica B*158:291, 1989.
306. J. D. Bozek, J. N. Cutler, G. M. Bancroft, and J.S. Tse. Variable energy photoelectron study of the valence levels of CF₃Cl and CF₃Br. *Chem.Phys.* 132:257, 1989.
307. D. D. Klug, Y. P. Handa, J.S. Tse, and E. Whalley. Transformation of ice VIII to amorphous ice by "melting" at low temperatures. *J.Chem.Phys.* 90:2390, 1989.
308. T. K. Sham, B. X. Yang, J. Kirz, and J.S. Tse. Near edge X-ray absorption fine structure of oxygen and carbon containing molecules in the gas phase. *Phys.Rev.* A40:652, 1989.
309. J.S. Tse, Z. F. Liu, J. D. Bozek, and G. M. Bancroft. MSX α study of the silicon and chlorine core levels photoelectron spectra of SiCl₄. *Phys.Rev.A* 39:1791, 1989.
310. J.S. Tse. The d and f resonances in the core level absorption spectra of TeF₆. *Chem.Phys.Lett.* 163:392, 1989.
311. J.S. Tse and H. Morris. Ab initio study of the stability of Al--C₂H₄ adducts. *J.Chem.Soc.Chem.Comm.* 78, 1989.
312. D. S. Yang, G. M. Bancroft, R. J. Puddephatt, J. D. Bozek, and J.S. Tse. Assignment of the valence molecular orbital of cis-[PtR₂L₂] complexes: UV photoelectron spectra and SCF--MS--X α calculations. *Inorg.Chem.* 28:1, 1989.
313. F. L. Lee, E. J. Gabe, J.S. Tse, and J. A. Ripmeester. Crystal structure, CP/MAS ¹²⁹Xe and ¹³C NMR of local ordering in Dianins compound clathrates. *J.Am.Chem.Soc.* 110:6014, 1988.
314. B. Mile, J. A. Howard, and J.S. Tse. EPR studies of the addition of aluminium and gallium atoms to allene : a rule for regioselectivity. *Organometallics* 7:1278, 1988.
315. J. A. Ripmeester, C. I. Ratcliffe, and J.S. Tse. The NMR of ¹²⁹Xe trapped in clathrates and some other solids. *J.Chem.Soc.Faraday Trans.I*84:3731, 1988.
316. J. A. Ripmeester, M. A. Desando, Y. P. Handa, and J.S. Tse. Thermally induced phase transitions in the clathrasil dodecasil-3C (Zeolite ZSM-39). *J.Chem.Soc.Chem.Comm.* 608, 1988.
317. J.S. Tse and M. L. Klein. A molecular dynamics study of the effect of pressure on the properties of water and ice. *J.Phys.Chem.* 92:315, 1988.
318. J.S. Tse and M. A. White. The origin of the glassy crystalline behaviour in the thermal properties of clathrate hydrates : a thermal conductivity study of tetrahydrofuran hydrate. *J.Phys.Chem.* 92:5006, 1988.
319. J.S. Tse. Electronic structure of the dimer and trimer of aluminium. *Theo.Chem.* 165:21, 1988.
320. J.S. Tse. Resonant enhancement in the valence orbital photoionization cross sections of XeF₂. *J.Chem.Phys.* 89:920, 1988.
321. G. M. Bancroft, S. Aksela, H. Aksela, K. Gürtler, K. H. Tan, B. W. Yates, and J.S. Tse. Photoelectron study of the valence level cross sections of XeF₂ above the Xe 4d threshold: many body effect. *J.Phys.B*B20:3057, 1987.
322. J. E. Bice, K. H. Tan, G. M. Bancroft, and J.S. Tse. A variable energy photoelectron study of the valence levels of Si(CH₃)₄ and Sn(CH₃)₄ and the Sn 4d levels of Sn(CH₃)₄. *Inorg.Chem.* 26:4106, 1987.
323. J. E. Bice, K. H. Tan, G. M. Bancroft, B. W. Yates, and J.S. Tse. A variable energy photoelectron study of the valence and Hg 5d levels of Hg(CH₃)₂. *J.Chem.Phys.* 87:821, 1987.
324. J. D. Bozek, K. H. Tan, G. M. Bancroft, and J.S. Tse. Gas phase photoabsorption spectra of SiCl₄ and Si(CH₃)₄ at the silicon K edges : characterization and assignment of resonances. *Chem.Phys.Lett.* 138:33, 1987.
325. D. W. Davidson, J. A. Ripmeester, and J.S. Tse. Some structural studies on clathrate hydrates. *J.de Phys.Colloque C1 Supplement* 48:537, 1987.
326. D. W. Davidson, M. A. Desando, S. R. Gough, Y. P. Handa, C. I. Ratcliffe, J. A. Ripmeester, and J.S. Tse. Some physical and thermophysical properties of clathrate hydrates. *J.Incl.Phenom.* 5:219, 1987.
327. D. W. Davidson, S. R. Gough, Y. P. Handa, C. I. Ratcliffe, J. A. Ripmeester, and J.S. Tse. some structural studies of clathrate hydrates. *J.de Phys.Colloque* 48:C1-537, 1987.

328. D. W. Davidson, M. A. Desando, S. R. Gough, Y. P. Handa, C. I. Ratcliffe, J. A. Ripmeester, and **J.S. Tse**. A clathrate hydrate of carbon monoxide. *Nature* 328:418, 1987.
329. J. A. Howard, B. Mile, **J.S. Tse**, and H. Morris. The EPR spectrum of Al(C₂H₄) in hydrocarbon matrices. *J.Chem.Soc.Faraday Trans.I*83:3701, 1987.
330. M. Marchi, **J.S. Tse**, and M. L. Klein. Infrared and raman spectra of hexagonal ice in the lattice mode region. *J.Chem.Soc.Faraday Trans.II*83:1867, 1987.
331. J. R. Morton, K. F. Preston, A. Sayari, and **J.S. Tse**. Reactions of a paramagnetic silver cluster with NH₃ and C₂H₄. *J.Phys.Chem.* 91:2117, 1987.
332. J. A. Ripmeester, **J.S. Tse**, C. I. Ratcliffe, and B. M. Powell. A new clathrate hydrate structure. *Nature* 325:135, 1987.
333. **J.S. Tse**. Thermal expansion of the clathrate hydrates of ethylene oxide and tetrahydrofuran. *J.de Phys.* C1:543, 1987.
334. **J.S. Tse**, R. E. McKinnon, and M. Marchi. Thermal expansion of the structure I clathrate of ethylene oxide. *J.Phys.Chem.* 91:4108, 1987.
335. **J.S. Tse** and M. L. Klein. Molecular dynamics studies on the pressure induced order → amorphous transitions in ice I_h. *Phys.Rev.Lett.* 58:1682, 1987.
336. **J.S. Tse** and M. L. Klein. Molecular dynamics calculation of the infrared and raman spectra of Ice IX in the translational mode region. *Chem.Phys.Lett.* 142:175, 1987.
337. **J.S. Tse** and M. L. Klein. Dynamical properties of the structure II hydrate of krypton. *J.Phys.Chem.* 91:5789, 1987.
338. G. M. Bancroft, S. Aksela, H. Aksela, K. H. Tan, B. W. Yates, L. L. Coatsworth, and **J.S. Tse**. Shape resonance above the Si 4p threshold in SiF₄. *J.Chem.Phys.* 84:5, 1986.
339. G. M. Bancroft and **J.S. Tse**. Ligand field splittings on core levels of main group compounds and metal surfaces from photoelectron spectroscopy. *Comment Inorg.Chem.* 5:89, 1986.
340. D. W. Davidson, S. K. Garg, Y. P. Handa, C. I. Ratcliffe, S. R. Gough, J. A. Ripmeester, **J.S. Tse**, and W. F. Lawson. Laboratory analysis of a naturally occurring gas hydrate from sediment of the Gulf of Mexico. *Geochim.Cosmochim.Acta* 50:619, 1986.
341. D. W. Davidson, Y. P. Handa, C. I. Ratcliffe, J. A. Ripmeester, **J.S. Tse**, J. R. Dahn, F. L. Lee, and L. D. Calvert. Crystallographic studies of clathrate hydrates. Part I. *Mol.Cryst.Liq.Cryst.* 141:141, 1986.
342. Y. P. Handa and **J.S. Tse**. Thermodynamical properties of empty lattices of structure I and structure II clathrate hydrates. *J.Phys.Chem.* 90:5917, 1986.
343. M. Marchi, **J.S. Tse**, and M. L. Klein. Lattice dynamics and infrared absorption of ice I_h. *J.Chem.Phys.* 85:2414, 1986.
344. **J.S. Tse** and J. D. Goddard. The electronic structure of trifluoronitrosomethane. *Theo.Chem.* 139:165, 1986.
345. **J.S. Tse**, Y. P. Handa, C. I. Ratcliffe, and B. M. Powell. Structure of oxygen clathrate hydrate by powder neutron diffraction. *J.Incl.Phenom.* 4:235, 1986.
346. **J.S. Tse**. Electronic structures of the mono- and tri-carbonyl of Cu and Ag. *Ber.Bunsenges.phys.Chem.* 90:906, 1986.
347. **J.S. Tse**, M. J. Collins, F. L. Lee, and E. J. Gabe. Crystal, molecular and electronic structure of methyltin triiodide. *J.Org.Chem.* 310:169, 1986.
348. **J.S. Tse**, F. L. Lee, and E. J. Gabe. Room temperature and low temperature crystal and molecular structure of triphenyltin chloride. *Acta Crystallogr.C*42:1875, 1986.
349. B. W. Yates, G. M. Bancroft, K. H. Tan, and **J.S. Tse**. A variable energy photoelectron study of the valence levels and I 4d core levels of CF₃I. *J.Chem.Phys.* 85:3840, 1986.
350. G. I. Birnbaum, D. D. Klug, J. A. Ripmeester, and **J.S. Tse**. The crystal structure and infrared spectrum of an inclusion compound of cyclotrimeratrylene and water. *Can.J.Chem.* 63:3258, 1985.
351. J. B. Chenier, J. A. Howard, **J.S. Tse**, and B. Mile. An ESR study of the reaction of aluminium atoms with buta-1,3-diene: cheletropic cycloaddition and substituted allyl formation. *J.Am.Chem.Soc.* 107:7290, 1985.

352. J. A. Howard, R. Sutcliffe, **J.S. Tse**, H. Dahmane, and B. Mile. Electron spin resonance spectra of aluminium trimer in hydrocarbon matrices: a quartet 4A_2 state. *J.Phys.Chem.* 89:3595, 1985.
353. C. I. Ratcliffe, J. A. Ripmeester, and **J.S. Tse**. NMR chemical shifts of dilute 1H in inorganic solids. *Chem.Phys.Lett.* 120:427, 1985.
354. **J.S. Tse**, E. Pellach, and G. M. Bancroft. Experimental and theoretical shakeup studies VI. The fluoromethanes. *Can.J.Chem.* 63:457, 1985.
355. B. W. Yates, K. H. Tan, G. M. Bancroft, L. L. Coatsworth, and **J.S. Tse**. Photoelectron study of the valence levels of CF_4 and SiF_4 from 20eV to 100eV. *J.Chem.Phys.* 83:4906, 1985.
356. D. W. Davidson, S. K. Garg, S. R. Gough, Y. P. Handa, C. I. Ratcliffe, **J.S. Tse**, and J. A. Ripmeester. Some structural and thermodynamic studies of clathrate hydrates. *J.Incl.Phenom.* 2:231, 1984.
357. D. W. Davidson, S. K. Garg, C. I. Ratcliffe, **J.S. Tse**, and S. R. Gough. Characterization of a clathrate hydrate of nitrogen trifluoride. *Can.J.Chem.* 62:1229, 1984.
358. D. W. Davidson, Y. P. Handa, C. I. Ratcliffe, **J.S. Tse**, and B. M. Powell. The ability of small molecules to form clathrate hydrates of structure II. *Nature* 311:142, 1984.
359. J. A. Howard, R. Sutcliffe, **J.S. Tse**, and B. Mile. Cryochemical Studies 11. ESR studies of the reaction of Group 1B metal atoms with some mono and disubstituted acetylenes in a rotating cryostat. *Organometallics* 3:859, 1984.
360. R. W. Impey, M. L. Klein, and **J.S. Tse**. Effective potentials and the structure of ices VIII and IX. *J.Chem.Phys.* 81:6406, 1984.
361. S. Larsson, **J.S. Tse**, J. L. Esquivel, and A. T. Kai. Electronic structure and ESCA shakeup of the UF_6 molecule. *Chem.Phys.* 89:43, 1984.
362. **J.S. Tse**, E. Pellach, and G. M. Bancroft. The He I and He II photoelectron spectra of VOF_3 and $VOCl_3$. *Inorg.Chim.Acta* 83:93, 1984.
363. **J.S. Tse**, M. L. Klein, and I. R. McDonald. Computer simulation studies of the structure I clathrate hydrates of methane, tetrafluoromethane, cyclopropane and ethylene oxide. *J.Chem.Phys.* 81:6146, 1984.
364. **J.S. Tse**, M. L. Klein, and I. R. McDonald. Lattice vibrations of ices I_h , VIII and IX. *J.Chem.Phys.* 81:6124, 1984.
365. G. M. Bancroft, D. J. Bristow, **J.S. Tse**, and G. Schrobilgen. Theoretical and experimental shake-up studies of KrF_2 . *Inorg.Chem.* 22:2673, 1983.
366. D. J. Bristow, G. M. Bancroft, and **J.S. Tse**. High resolution (He I & II) photoelectron spectra of the zinc and cadmium dihalides valence band. *Chem.Phys.* 75:263, 1983.
367. D. J. Bristow, **J.S. Tse**, and G. M. Bancroft. High resolution (He I & II) photoelectron spectra of the Zn 3d and Cd 4d orbitals in the zinc and cadmium dihalides. *Chem.Phys.* 75:277, 1983.
368. J. A. Howard, R. Sutcliffe, **J.S. Tse**, and B. Mile. ESR spectrum of paramagnetic copper (Cu_5). A trigonal bipyramidal copper cluster. *Chem.Phys.Lett.* 94:561, 1983.
369. C. I. Ratcliffe, J. A. Ripmeester, and **J.S. Tse**. ^{15}N NMR chemical shifts in solid NH_4^+ salts. *Chem.Phys.Lett.* 99:177, 1983.
370. **J.S. Tse**, M. L. Klein, and I. R. McDonald. Molecular dynamics of ice I_c and the structure I clathrate hydrate of methane. *J.Phys.Chem.* 87:4198, 1983.
371. **J.S. Tse**, M. L. Klein, and I. R. McDonald. Dynamical properties of structure I clathrate hydrate of xenon. *J.Chem.Phys.* 78:2096, 1983.
372. **J.S. Tse** and J. A. Ripmeester. Experimental and theoretical studies on the charge-transfer transition in SO_2 - β -quinol and related complexes. *J.Phys.Chem.* 87:1708, 1983.
373. **J.S. Tse** and M. L. Klein. Are hydrogen atoms solvated by water molecules? *J.Phys.Chem.* 87:5055, 1983.
374. L. P. Aldridge, **J.S. Tse**, and G. M. Bancroft. Extended Hückel calculation of Fe^{2+} electronic energies in silicates -- amphipole electronic spectra revisited. *Am.Mineral.* 67:335, 1982.

375. G. M. Bancroft, E. Pellach, and J.S. Tse. High resolution (He I & He II) photoelectron spectra of TiCl_4 , SnCl_4 and $(\text{CH}_3)_4\text{Sn}$. *Inorg.Chem.* 21:2950, 1982.
376. G. M. Bancroft, T. Chan, R. J. Puddappatt, and J.S. Tse. The role of the Au 5d orbitals in bonding: The photoelectron spectra of $[\text{AuMe}(\text{PMe})_3]$. *Inorg.Chem.* 21:2946, 1982.
377. D. J. Bristow, J.S. Tse, and G. M. Bancroft. Theoretical and experimental shakeup studies: Part V, shakeup in rare gases. *Phys.Rev.* A25:1, 1982.
378. S. K. Garg and J.S. Tse. Ab initio quantum mechanical calculation of ^{13}C , ^{15}N and ^{19}F chemical shifts in CF_3X ($\text{X}=\text{H},\text{F},\text{CN},\text{Cl},\text{NO}$). *Chem.Phys.Lett.* 92:150, 1982.
379. J. A. Ripmeester, J.S. Tse, and D. W. Davidson. ^{13}C NMR characterization of acetonitrile hydroquinone clathrate. *Chem.Phys.Lett.* 86:428, 1982.
380. J.S. Tse and D. W. Davidson. Intermolecular potential for gas hydrates. *Proc.of 4th Cdn.Permafrost Conference* :329, 1982.
381. J.S. Tse. Theoretical studies of magnetic shielding in HCN and $(\text{HCN})_2$. *Chem.Phys.Lett.* 92:144, 1982.
382. J.S. Tse, D. K. Creber, and G. M. Bancroft. Theoretical and experimental shakeup studies: Part IV, main group Me_2M ($\text{M}=\text{Zn},\text{Cd},\text{Hg}$) compounds. *J.Chem.Phys.* 74:2097, 1981.
383. J.S. Tse and G. Loubriel. Theoretical calculation of shakeup intensities using $X\alpha$ -SW wave functions. *J.Chem.Phys.* 74:5190, 1981.
384. J.S. Tse. A SCF- $X\alpha$ - SW study of the shakeup in TiCl_4 . *Chem.Phys.Lett.* 77:373, 1981.
385. D. K. Creber, J.S. Tse, and G. M. Bancroft. Experimental and theoretical shakeup studies: Part III. The 1s shakeup in CH_4 , NH_3 and H_2O . *J.Chem.Phys.* 72:4291, 1980.
386. R. P. Gupta, J.S. Tse, and G. M. Bancroft. Core level ligand field splittings in the photoelectron spectra. *Phil.Trans.Roy.Soc.* 293A:535, 1980.
387. J.S. Tse and G. M. Bancroft. Broadening of the Ba $5p_{3/2}$ Level in the Photoelectron Spectra of the Barium Halides. *Chem.Phys.Lett.* 69:479, 1980.
388. J.S. Tse. Calculation of single orbital relaxation accompanying core ionization in the isoelectronic ten electron hydrides by the $X\alpha$ SW method. *J.Chem.Phys.* 73:3015, 1980.
389. J.S. Tse. Theoretical calculation of multiplet structures in shakeup spectra by the $X\alpha$ method. *J.Chem.Phys.* 73:5734, 1980.
390. J.S. Tse, T. K. Sham, and G. M. Bancroft. Stereochemistry of six coordinated organotin(IV) compounds with bidentate ligands. *Can.J.Chem.* 57:2223, 1979.
391. J.S. Tse, D. J. Bristow, G. M. Bancroft, and G. Schrobilgen. Theoretical and experimental shakeup studies on the Xe Core Level ESCA of XeF_2 . *Inorg.Chem.* 18:1766, 1979.
392. R. P. Gupta, J.S. Tse, and G. M. Bancroft. Role of the Sternheimer effect in the ligand field splittings of nuclear and electronic levels. *J.Chem.Phys.* 68:4192, 1978.
393. T. C. W. Mak and J.S. Tse. A computer program for generating atom positions. *Quantum Chemistry Program Exchange Catalogue* No. 345, 1978.
394. G. M. Bancroft, D. K. Creber, and J.S. Tse. High resolution core level photoelectron spectroscopy using He II radiation. Electric field gradient splittings in group IIB and III compounds. *Chem.Phys.Lett.* 50:288, 1977.
395. G. M. Bancroft, L. L. Coatsworth, D. K. Creber, and J.S. Tse. High resolution gas phase photoelectron spectra of core d level using He II radiation. *Phys.Scr.* 16:217, 1977.
396. T. L. Chan, K. W. Ho, C. K. Chan, J.S. Tse, and T. C. W. Mak. Synthesis and x-ray structure of 2,11 dithia-6,15-dimethyl (3.3) metacyclophane. *J.Cryst.Mol.Struct.* 7:199, 1977.
397. T. K. Sham, J.S. Tse, and G. M. Bancroft. Preparation and Mössbauer spectra of organotin(IV) compounds containing the $\text{CH}_3(\text{C}_6\text{H}_5)\text{Sn}(\text{IV})$ moiety. *Can.J.Chem.* 55:3487, 1977.
398. T. C. W. Mak, J.S. Tse, C. S. Tse, K. S. Lee, and Y. K. Chong. Crystal structure of a clathrate inclusion compound of hydroquinone and hydrogen sulphide. *J.Chem.Soc.Perkin Trans.* II:1169, 1976.
399. J.S. Tse and T. C. W. Mak. Refinement of the crystal structure of polyethylene terephthalate. *J.Cryst.Mol.Struct.* 5:75, 1975.