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THEORETICAL STUDIES ON THE ELECTRONIC STRUCTURE
AND PROPERTIES OF COMPLEX CERAMIC CRYSTALS AND GLASSES

Annual Progress Report
for Period July 1, 1989 - June 30, 1990

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Summary

This report summarizes the research activities for the period 7/1/89 - 6/30/90 under the DOE grant DE-FG02-84ER45170. This is the last year of a three-year project started July 1, 1986. A new three year renewal proposal was submitted on September 10, 1989 and was approved by the Department of Energy. In that proposal, the research accomplishments of the past three years were summarized. This report contains that section of the renewal proposal describing the major accomplishments which are listed under the following subject headings:

(a) Electronic structures and properties of ceramic crystals. (b) Theory of high T_c superconductors. (c) Total energy and structural phase transitions. (d) Properties of Re-Fe-B magnetic system. (e) Basic study on metallic glasses. (f) Basic study on insulating glasses. In addition, further accomplishments and activities in the most recent six months are also described.

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I. Introduction.

This annual report covers the last year of a three-year project supported by the Department of Energy that was started on July 1, 1986. Within these three years, a phenomenal amount of research results have been obtained. These accomplishments were fully documented in a renewal proposal sent to the Department of Energy on September 10, 1989. This three-year renewal proposal has been approved by the Office of Basic Energy Research of DOE and will start on July 1, 1990.

In the following section, Section II, we summarize the research work accomplished since July 1, 1986 as was documented in the renewal proposal. In Section III, we list additional accomplishments since the submission of the renewal proposal. Section IV contains the figures that have been referred to in Section II. In Section V, we list the scientific personnel and students that have been involved in the project. Technical papers published or submitted under the DOE support since the last annual report are documented in Section V. Because of the large number of papers published or submitted, reprint and preprint copies will be submitted separately instead of attaching in the form of appendix.

II. Summary of Work Accomplished (7/1/86-9/1/89)

This section summarizes our research accomplishments under the DOE support for the period 7-1-1987 to 6-30-1990 which include some of the work currently in progress. They are broadly divided into six major categories not necessarily in the order of importance. In order to keep this proposal concise and succinct, we will only stress the significant aspects of each subject and leave the detailed information to the published papers which are listed in a chronological order in the publication list (PL) of the Principal Investigator. More recent results are illustrated and discussed.

(a) Electronic structures and properties of ceramic crystals.

The electronic structures of complex ceramic crystals have been extensively studied by our group. For more than a decade, we have developed and refined the orthogonalized linear combination of atomic orbitals method (OLCAO) to make it an accurate, state-of-the-art method for electronic structure calculations. The method is suited to any condensed matter system, but is particularly powerful for complex systems where other methods may not be convenient. Self-consistent band structures have been obtained for the following ceramic systems: AlN, α -SiO₂, β -Si₃N₄, ZrO₂, Cu₂O, CuO, YBa₂Cu₃O₇ [1-2-3], F-substituted YBa₂Cu₃O₇, Zn- and Ga- substituted YBa₂Cu₃O₇ and other recently discovered high temperature superconductors. Currently we are studying the electronic structures of α -Al₂O₃, MgO, tetragonal and monoclinic phases of ZrO₂ and all other polycrystalline forms of SiO₂ such as β -quartz, tridymite, α - and β -cristobalite, coesite, keatite, and stishovite. The significance of

these studies is that most of these materials have very complicated structures and an accurate electronic structure calculation is a nontrivial task. Fig. 1 shows the self consistent band structure of $\alpha\text{-Al}_2\text{O}_3$ which has a complicated corundum structure. Previously, only a non-selfconsistent calculation has been performed. Based on the electronic structure results, other physical observables can be studied. We have studied the linear optical properties of most of the above ceramic crystals with very good agreement with the available experimental measurements. Calculations of optical properties of Cu_2O resulted in a complete reinterpretation of some of the experimental data of long standing. Fig. 2 shows the calculated imaginary part of the dielectric function of $\alpha\text{-Al}_2\text{O}_3$ up to 40. eV which compares well with the recent experimental data from DuPont research laboratory. Fig. 3 shows a similar calculation for crystalline $\beta\text{-Si}_3\text{N}_4$. The calculated optical conductivity curve is compared with the experimental data for amorphous Si_3N_4 . The agreement has been excellent both in the position and the magnitude of the major peak. We have also studied the optical properties of high T_c superconductors ($\text{YBa}_2\text{Cu}_3\text{O}_7$, substitutions of Zn and Ga in $\text{YBa}_2\text{Cu}_3\text{O}_7$, Bi-1222, Tl-2122 and Tl-2223 superconductors). Our study has added to a deeper understanding of these fascinating materials and facilitated the formulation of plausible theoretical models. The band structures of $\text{YBa}_2\text{Cu}_3\text{O}_7$ and those with substitution of Cu(1) site by Zn and Ga are illustrated in Fig. 4.

(b) Theory of high T_c superconductors.

(in Collaboration with K. W. Wong, University of Kansas)

Based on the earlier work of Wong on a certain class of semiconductors using many body theory and the results of electronic structures and optical conductivity calculations on the high T_c superconductors, we have formulated an excitonic enhancement model (EEM) of superconductivity. This theory advocates a simultaneous excitonic-superconductivity condensation of charge non-neutral quasi particles and is formulated from two different points of view: (1) By assuming a strong Coulomb binding between electrons in the empty conduction band and the intrinsic hole population in the valence band, and then deriving a total excitation gap in the mean-field approximation as a Pythagorean sum of excitonic and BCS gap components; (2) as a manifestation of the off-diagonal-long-range ordering of quasi particles due to a strong electron-hole correlation.

A variety of experimental observations appear to be consistent with the EEM model. Among them are the explanation of double specific heat jump at T_c for the [1-2-3] compound, the weak isotope dependence of T_c , far infra-red optical spectra and positron annihilation data etc. Recently, it has been shown that excitonic binding in two dimensions will be enhanced by a factor of 4 over that of the 3-dimension. This fact makes the EEM theory even more plausible for the highly anisotropic high T_c superconductors. A lot remains to be done in terms of formal analytical theory and more accurate numerical calculations on other well-characterized high T_c superconducting and related non-superconducting phases in order to check the validity of this theory.

(c) Total energy and structural phase transitions.

The accuracy of total energy calculation with the OLCAO method has been demonstrated in Si and AlN . Results on the equilibrium volume, bulk modulus B , the pressure derivative of B and some optical phonon modes are in excellent agreement with experiment. Preliminary calculations have also been done for α -SiO₂ and β -Si₃N₄ with very encouraging results. In order to be able to study structural phase transitions in complex ceramic crystals, we must demonstrate that our method is of sufficient accuracy for such a purpose. A good testing ground is Si with which the first-principles pseudopotential method has been extremely successful. We have performed the total energy calculation on Si as a function of lattice parameters in several different crystal structures using the OLCAO method. The phases studied include the cubic diamond(c-dl), the hexagonal diamond(hex), the β -tin, the simple hexagonal(sh), and the hcp, fcc, bcc, sc and bc8 structures. The calculated total energy curves for all the phases are shown in fig.5. The phase transformation curves from the c-dl to β -tin; β -tin to sh; sh to hcp and hcp to fcc are shown in fig. 6. The calculated transition pressures and volumes are in good agreement with experimental values. The overall result on the pressure-induced structural phase transformations in Si is very close to that obtained by the UC-Berkeley group using the pseudopotential method.

While total energy calculations using local density theory become quite routine in recent years, its application to structural phase transitions has been limited to crystals with simple structures. We intend to carry out the same type of calculation for complex ceramic systems such

as ZrO_2 , SiO_2 and Si_3N_4 .

(d) Properties of Re-Fe-B magnetic system.

Immediately after the discovery of the R-Fe-B (R= rare earth) compounds with their outstanding permanent magnetic properties, our group has been involved in the study of its electronic and magnetic properties. Although there has been numerous experimental studies on these materials, theoretical efforts lag far behind. As a matter of fact, our group is probably the only one making sustained theoretical contributions in this area. $\text{R}_2\text{Fe}_{14}\text{B}$ is a tetragonal crystal of low symmetry containing a total of 68 atoms in the unit cell. The presence of localized f-electrons in the rare earth atoms poses a considerable challenge to the itinerant electron band theory. We have calculated the electronic structures of $\text{Y}_2\text{Fe}_{14}\text{B}$, $\text{Nd}_2\text{Fe}_{14}\text{B}$, $\text{Y}_2\text{Co}_{14}\text{B}$ and $\text{Nd}_2\text{Co}_{14}\text{B}$ using the OLCAO method including spin polarization (non-selfconsistent). The calculation has also been extended to $\text{Gd}_2\text{Fe}_{14}\text{B}$ and Co- substituted $\text{Y}_2\text{Fe}_{14}\text{B}$. Results on the total density of states (DOS) as well as orbital-projected, spin-projected, and site-projected, partial DOS are obtained. These are illustrated in fig.7 for $\text{Nd}_2\text{Fe}_{14}\text{B}$. The spin magnetic moments on the transition metal sites are found to be in good agreement with the neutron- scattering data. The spin density in the [110] plane shows a network type of structure which could be related to its superior permanent magnetic properties.

Recently, using real space charge distribution calculated from the band structure, we have calculated the crystal-field parameters (CFP) at the Nd site in $\text{Nd}_2\text{Fe}_{14}\text{B}$ from first- principles (beyond the point charge model). Our results are in good agreement with experiments and have

clarified some wrong concepts attributed to the inaccurate CFP calculated by the point charge model. The CFP obtained are then used to construct a magnetic hamiltonian based on which the zero temperature crystal anisotropic energy is estimated, and is found to be consistent with experimental data. We are currently investigating the contribution from the orbital moments to total magnetization in $\text{Nd}_2\text{Fe}_{14}\text{B}$ using the same band structure results.

(e) Basic study on metallic glasses.

In the past few years, our group has been engaged in a basic study of metallic glasses. Metallic glasses prove to be a very fertile area to study many fascinating physics unique to disordered systems. Electronic structures of several important metallic glass systems have been studied by the OLCAO method. The calculation starts with the construction of large periodic models containing 100-200 atoms in the unit cell by Monte Carlo relaxation method using pair-wise interatomic potentials. Our study covers different types of metallic glasses, transition-metal - transition metal glass ($\text{a-Cu}_{1-x}\text{Zr}_x$), metastable amorphous Ni, transition metal-metalloid glass ($\text{a-Ni}_{1-x}\text{P}_x$), and free-electron like glass ($\text{a-Mg}_{1-x}\text{Zn}_x$). The interatomic potentials used in the model construction have also been utilized to study the vibrational dynamics in these glasses. The calculated DOS curves together with the localization index for $\text{a-Mg}_{70}\text{Zn}_{30}$ and $\text{a-Cu}_{60}\text{Zr}_{40}$ are illustrated in fig. 8.

More recently, we have succeeded in performing first principles transport calculations on metallic glasses. The energy dependent conductivity function $\sigma(E)$ is obtained from the direct evaluation of the

Kubo-Greenwood formula without any approximation to the dipole transition matrix elements. Fig. 9 shows the calculated $\sigma(E)$ curves of $a\text{-Mg}_{1-x}\text{Zn}_x$ and $a\text{-Cu}_{1-x}\text{Zr}_x$ near the Fermi level. The calculated zero temperature resistivity values and thermo power are in good agreement with experiments. This is illustrated in Fig. 10. We find that at low temperature, the transport properties are controlled by the magnitude and the shape of the conductivity function near the Fermi level. We also conclude that at low temperature, elastic scattering of the conduction electrons from the disordered atoms alone is sufficient to account for the negative temperature coefficient observed in many metallic glass systems. The Mooij correlation can be naturally explained in terms of the competition between this effect and the positive contribution to the resistivity from the electron-phonon scattering. The origin of this can be traced to the fact that the Fermi Energy (E_F) happens to locate at a local minimum in the conductivity curve. The existence of a minimum at E_F in the $\sigma(E)$ curve may also be related to the relative stability of the glass against local configurational fluctuations. Our results seem to be consistent with the theory of quantum coherence or weak localization of disordered solids. We consider our first-principles studies of transport properties of metallic glasses to be highly significant and will have a far-reaching effect on the theory of disordered systems. Calculations of optical properties of some of these systems have also been performed with results in reasonable agreement with experiments.

(f) Basic study on insulating glasses.

Periodic models have been used to study the electronic structures of

a-SiO_2 and $(\text{SiO}_2)_{1-x}(\text{Na}_2\text{O})_x$ glasses in the past. We have used the same models to study the vibrational, infrared and Raman spectra in a-SiO_2 . The periodic models for the insulating glasses are much more difficult to construct than the metallic glasses because of the directional bonding involved in the covalent or partially covalent systems. We used a Keating-type of potential for the relaxation process and for obtaining the dynamic matrix. The vibrational density of states are obtained by direct diagonalization of the dynamic matrix and the infra-red and the Raman spectra are calculated following the approach of Bell and Dean. The spectra compare favorably with experimental data. Our calculation supports the random continuous network model for the structure of a-SiO_2 and we argue against the para-crystalline model. This is based on the fact that our calculation reproduced the two Raman lines at 495 and 606 cm^{-1} which were previously attributed to surface related non-binding oxygen sites. The occurrence of these modes is traced to the atoms with specific Si-O-Si bonding angles, rather than simply the number of Si atoms in a closed ring as suggested by Galeener.

By compressing the model structure and re-relaxing under the same potential, new models of a-SiO_2 under hydrostatic pressure are obtained. We have utilized these models to study the pressure dependence of the infra-red and Raman spectra in a-SiO_2 . The results are illustrated in fig. 11.

For a more realistic study of basic properties of insulating glasses, we need to develop more accurate potential models beyond the Keating model. First-principles total energy and structural phase

transition calculations on a few selected ceramic crystals described in
(c) will facilitate the construction of better potential functions.

III. Summary of accomplishment in the most recent six months of the current year. (10/1/89-6/30/90)/90)

Additional accomplishments during the last six months are now briefly listed below:

(1) Development of relativistic corrections to the OLCAO method. This includes the scalar relativistic correction as well as spin-orbit interaction.

(2) Development of spin-polarized version of the OLCAO method for study of magnetic materials and for the inclusion of spin-orbit interaction. The method has been applied to the ferromagnetic compounds FeB, Fe_2B and Fe_3B .

(3) Study of electronic and optical properties of certain ceramic compounds such as Y_2O_3 , $\alpha\text{-Al}_2\text{O}_3$, MgO, and the spinel MgAl_2O_4 . Nonlinear optical crystals such as LiB_3O_5 and KTiOPO_4 (KTP).

(4) Continuation and extension of total Energy studies to the different phases of ZrO_2 and BN. Techniques to further improve the accuracy and speed for total energy calculation are also under development.

(5) A comprehensive review article entitled "Theoretical Studies of the Electronic Properties of Ceramic Materials" is being prepared and will be published in the Journal of the American Ceramic Society. This manuscript which is in excess of 100 pages is now near completion. It provides a detailed account of the theory and the method for basic studies of the ceramic materials, and also the work accomplished by our group at the University of Missouri-Kansas City under the DOE support.

IV. Figure captions and Figures

Fig.1 Electronic structure of trigonal $\alpha\text{-Al}_2\text{O}_3$: (a) band structure; (b) density of states.

Fig.2 (a) Calculated frequency dependent dielectric function of $\alpha\text{-Al}_2\text{O}_3$; (b) recent experimental data (ref.4) from a group at DuPont. The shaded peak is due to that of an exciton.

Fig.3 (a) The selfconsistent band structure of $\beta\text{-Si}_3\text{N}_4$. (b) The optical conductivity of $\beta\text{-Si}_3\text{N}_4$. The circles are the experimental data for amorphous Si_3N_4 from reference 5.

Fig.4 (a) Band structure of $\text{YBa}_2\text{Cu}_3\text{O}_7$; (b) band structure of [1-2-3] with a Cu_1 site (on the chain) substituted by Zn; (c) band structure of [1-2-3] with a Cu_1 substituted by Ga.

Fig.5 Total energy of Si as a function of ratio to the volume of diamond Si for all possible crystal phases.

Fig.6 Calculated structural phase transitions in Si: (a) from d-Si to β -tin; (b) from β -tin to sh Si; (c) from sh Si to hcp Si; (d) from hcp Si to fcc Si.

Fig.7 Orbital-, spin- and site-projected partial density of states of $\text{Nd}_2\text{Fe}_{14}\text{B}$: Left panel: (a) Total DOS; (b) solid line, Nd 6s; dashed line, Nd 4f; (c) solid line, Fe 4s; dashed line, Fe 4p; dotted line, Fe 3d; (d) solid line B 2s; dashed line, B 2p. Right panel: Partial DOS at different Fe sites: (a) 4e, (b) 4c, (c) 8j1, (d) 8j2, (e), 16k1, (f), 16k2. Above zero is for the spin-up band and below zero is for the spin-down band.

Fig.8 DOS (left hand scale) and localization index (right hand scale)

calculated for 200-atom model of: (a) $a\text{-Mg}_{70}\text{Zn}_{30}$; (b) $a\text{-Cu}_{60}\text{Zr}_{40}$.

Fig.9 Conductivity function near Fermi level of (a) $a\text{-Mg}_{1-x}\text{Zn}_x$; (b) $a\text{-Cu}_{1-x}\text{Zr}_x$.

Fig.10 Calculated temperature dependent resistivity $\rho(T)$ of: (a) $a\text{-Mg}_{1-x}\text{Zn}_x$; (b) $a\text{-Cu}_{1-x}\text{Zr}_x$. The resistivity is due to elastic disorder scattering alone and does not include the contribution from the electron-phonon scattering.

Fig.11 Infrared absorption (upper panel) and Raman spectra (lower panel) for compressed models of $a\text{-SiO}_2$: (a) normal density, (b) 5% density increase, (c) 10% density increase, (d) 15% density increase, (e) 20% density increase.

Al₂O₃-Trigonal

Fig. 1

2

Fig. 2

Fig. 4

Fig. 6

Fig. 8

Fig. 9

Fig. 10

Fig. 11

V. Efforts of scientific personnel involved.

(1)	W.Y. Ching, Principal Investigator	
	25% academic year	not paid by the grant
	3 summer months	paid by the grant
(2)	Xue-Fu Zhong [*] , Research Associate	paid partly by the grant
	Yong-Nain Xu [#] , Research Associate	paid partly by the grant
(3)	Graduate Research Assistants:	
	Yi He ^{\$}	paid two months by the grant
	Farzlen Zandiehnam ⁺	paid by the grant
	F. Gan ^{&}	paid partly by the Grant
(4)	Visiting Scholar	
	Ming-Zhu Huang	not paid by the grant
(5)	Research Collaborator	
	Professor K.W. Wong	
	10% academic year	not paid by the grant
	1 summer month	paid by the grant
	(Visiting Research Professor)	

* Prof. Xue-Fu Zhong, a research associate of the DOE project since January 1, 1988 had returned to Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China in December, 1989.

Dr. Yong-nian Xu, who was a research associate on the DOE project earlier had returned to the University of Missouri-Kansas City on April 15, 1989. He replaces Prof. Zhong as a research associate for the DOE project starting January 1, 1990.

\$ Ms. He finished her M.S. Degree and is now meaningfully employed in Dallas, Texas.

+ Mr. Zandiehnam completed his Ph. D. degree and is now a post-doctoral fellow in the Chemistry Department of the University of Missouri-Kansas City.

& Mr. F. Gan joined as a new graduate research assistant in September, 1989. He replaces Mr. S. Weng who resigned earlier to seek industrial employment without completing the Ph. D. degree.

VI. List of scientific papers published, accepted and submitted.

(since last report)

(A) Work fully or partially supported by the project:

- 1.. "Electronic and Vibrational Structure Calculation on Models of the Compressed SiO₂ Glass System" (R. A. Murray and W.Y. Ching) Phys. Rev. B., 39, 1320 (1989).
2. "Comparative Study of Band Structures of Tl-Ca-Ba-Cu-O and Bi-Ca-Sr-Cu-O Superconducting Systems" (W.Y. Ching and Guan-Lin Zhao, Yong-nian Xu and K.W. Wong), Series on Progress in High Temperature Superconductivity, Vol. 12, p58 (1989) World Scientific. Edited by B.E. Baaquie, C. K. Chew, C. H. Lai, O. H. Oh and K.K. Phua.
3. "Interband Optical Conductivity of Bi₂CaSr₂Cu₂O₈ Superconductor, (W.Y. Ching, Guan-Lin Zhao, Y.-N. Xu and K.W. Wong) Modern Phys. Lett. B Vol 3, No 3, 263 (1989).
4. "Calculation of Interband Optical Conductivity of Tl₂CaBa₂Cu₂O₈ and Tl₂Ca₂Ba₂Cu₃O₁₀ Superconductors" (G.-L. Zhao, W.Y. Ching and K.W. Wong) J. of Optical Society of Am. B. Vol. 6, No. 3, 505 (1989).
5. "Theory of Simultaneous Excitonic and Superconductivity Condensation" (K.W. Wong and W.Y. Ching) Physica C, 158, 1 (1989).
6. "Theory of Simultaneous Excitonic and Superconductivity Condensation II: Experimental Evidences and Stoichiometric Interpretation" (K.W. Wong and W.Y. Ching) Physica C 158, 15 (1989).
7. "Microscopic Real-Space Approach to the Theory of Metallic Glasses." (G.-L. Zhao and W.Y. Ching) Phys. Rev. Lett. 62, 2511 (1989).
8. "Theoretical Differences in Fractional Charge Flux Quantization between the Anion Model and the Excitonic Enhancement Model for High T_c Superconductivity." (K.W. Wong and W.Y. Ching) Physics Lett. A. 136, 167 (1989).
9. "First-Principles Calculation of Crystal Field Parameters in Nd₂Fe₁₄B" (X.F. Zhong and W.Y. Ching) Phys. Rev. B. 39, 12018 (1989).
10. "Ground State and Optical properties of Cu₂O and CuO Crystals." (W.Y. Ching, Y.N. Xu and K.W. Wong) Phys. Rev. B. 40, 8111 (1989).
11. "First-Principles Calculation of Zero-temperature Anisotropic Energy in Nd₂Fe₁₄B." (X.F. Zhong and W.Y. Ching) Phys. Rev. B. (Rapid Communication) 40, 5292 (1989).
12. "Possibility of n-type and p-type Carrier Coupling in The Excitonic

- Enhancement Model of Superconducting Mechanism." (K.W. Wong and W.Y. Ching), Modern Phys. Letters B Vol. 4, 217 (1990).
13. "Ching replies to Muir's Comment." (W.Y. Ching) Phys. Rev. Letters, 64, 1181 (1990).
 14. "Realistic Calculation on the Second Order Nonlinear Susceptibility Tensor in Cubic Semiconductors." (W.Y. Ching and S. Weng) in Lattice Dynamics and Semiconductor Physics, World Scientific. Edited by J.B. Xia et. al. p 364, (1990)
 15. "Electronic Structure and Optical Properties of LiB_3O_5 Crystal." (Y.N. Xu and W.Y. Ching) Phys. Rev. B41, (Rapid Commun.), 5471 (1990)
 16. "Calculation of Local Orbital Moments of Conduction Electrons in $\text{Nd}_2\text{Fe}_{14}\text{B}$." (X.F. Zhong and W.Y. Ching), J. Appl. Phys., 67(9), 4768 (1990).
 17. "Orthogonalized Linear Combination of Atomic Orbitals Method. IV. Inclusion of Relativistic Effects." (X. F. Zhong, Y.-N. Xu and W.Y. Ching) Phys. Rev. B41, 10545 (1990).
 18. "Theory of Metallic Glasses, I: Electronic Properties." (W.Y. Ching G.-L. Zhao and Yi He) Phys. Rev. B. (Accepted)
 19. "Theory of Metallic Glasses, II: Transport and Optical Properties." (G.-L. Zhao, Yi He and W.Y. Ching) Phys. Rev. B. (Accepted)
 20. "Electronic Structures of Ga- and Zn- Substituted $\text{YBa}_2\text{Cu}_3\text{O}_7$ Superconductors" (Yong-nian Xu, W.Y. Ching and K.W. Wong) MRS Symposium M, High Temperature Superconductors: Fundamental Properties and Novel Materials Processing. (in Press)
 21. "Total Energy, Lattice Dynamics and Structural Phase Transition of Si by the Orthogonalized Linear Combination of Atomic Orbitals Method." (F. Zandiehnam and W.Y. Ching) Phys. Rev. B (Accepted)
 22. "Analytic Solution of Two-dimensional Hydrogen Atom. I. Non-relativistic Solution." (X.L. Yang, S.-H. Guo, F. T. Chan, K.W. Wong and W.Y. Ching) Submitted to Phys. Rev. A
 23. "Analytic Solution of Two-dimensional Hydrogen Atom. II. Relativistic Solution with Chern-Simon Action." (F.T. Chan, S.-H. Guo, X.L. Yang, K.W. Wong and W.Y. Ching) Submitted to Phys. Rev. A
 24. "The Optical Properties of Vanadium Pentoxide Determined From Ellipsometry Measurements and Band Structure Calculations." (J. C. Parker, D. J. Lam, Y.-N. Xu and W.Y. Ching) Submitted to Phys. Rev. B.
 25. "Electronic Structures of FeB , Fe_2B and Fe_3B Compounds by First-Principles Spin-polarized calculations", (W.Y. Ching, Y.-N. Xu,

B.N. Harmon, J. Yeh and C.T. Leung) Phys. Rev. B (Accepted).

26. "Selfconsistent Band Structures and Optical calculations in Cubic Ferroelectric Perovskites." (W.Y. Ching, Y.-N. Xu and R.H. French)
To appear in FERROELECTRICS.

(B) Scientific Work not directly related to the grant but representing
scholarly work in the general area of condensed matter theory.

(Supercomputer time allocated by Office of Basic Energy Research
may have been used in some cases)

1. "Field Enhanced Disorder in a Ferromagnet with Random Axis Anisotropy"
(D.L. Huber and W.Y. Ching) Phys. Rev. B 39, 4453 (1989).
2. "Harmonic Magnons in $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ and $\text{Zn}_{1-x}\text{Mn}_x\text{Te}$ " (T.M. Glebultowicz,
J.J. Rhyne, W.Y. Ching, D.L. Huber, J.K. Furdyna, B. Lebeck and R.R.
Galazica), Phys. Review B., 39, 6857 (1989).
3. "Numerical Simulation of the Optical Spectra of Frenkel Excitons in
Disordered Systems." (D.L. Huber and W.Y. Ching) Phys. Rev. B 39,
8652 (1989).
4. "Test of the Coherent Anisotropy Field Approximation for a Lattice
Model of Random Axis Ferromagnet in a High Magnetic Field." (D.L.
Huber and W.Y. Ching) Phys. Rev. B, 40, 2578 (1989).
5. "Simulation of the Optical Spectra Of Disordered Frenkel Excitonic
Systems by Equation-Of-Motion Techniques: Result for One Dimension."
(W.Y. Ching and D. L. Huber) J. of Luminensence 45, 335 (1990).
6. "Zero-Temperature Statics of a Random Exchange Model for the
Magnetic Properties of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$." (D.L. Huber and W.Y. Ching), J.
Appl. Phys., 67(9), 5743 (1990).
7. "Zero Temperature Statics and Dynamics of a Random Exchange Model
for the Magnetic Properties of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ in the Insulating Phase."
(W.Y. Ching and D. L. Huber) Phys. Rev. B (Accepted)
8. "Positron Annihilation Studies on the Tl-Ba-Ca-Cu-O Superconductors."
(C.S. Sundar, A.Bharathi, W.Y. Ching, Y.C. Jean, P.H. Hor, R.L. Meng,
Z.J. Huang and C.W. Chu), Submitted to Phys. Rev. B
9. "Studies of the Trapping of the Frekel Excitons in One Dimensional
Systems." (D.L. Huber and W.Y. Ching) to appear in Chemical Physics.

END

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