Georgia Tech Sponsored Research

Project	G-41-625	
Project director	Chou	Mei-Yin
Research unit	Physics	
Title	Presidential Young Investigator Award	
Project date	6/30/1999	

G-41-625

DMR-9157537 ANNUAL PROGRESS REPORT May, 1992
(10/1/91 - 9/30/92)

M. Y. Chou
School of Physics
Georgia Institute of Technology
Atlanta, GA 30332

SUMMARY OF RESEARCH

The objectives of my research are to investigate the electronic structure of condensed matter and to study its effects on the structural and dynamical properties of materials. The purpose of these studies is to provide unambiguous explanations for various interesting phenomena observed experimentally and to make reliable predictions of new material properties from microscopic quantum theories. Our efforts can be classified into two categories: (1) the study of the electronic and dynamical properties of particular systems (*a* and *b*) and (2) the development of new calculational algorithms and methods (*c* and *d*).

a. Hydrogen in Bulk Transition Metals

Hydrogen is the smallest and lightest interstitial impurity in transition metals. It interacts strongly with the metal host and behaves like a three-dimensional lattice gas with extremely high mobility. The diversity of phenomena exhibited by these systems (such as structural, order-disorder, and metal-semiconductor phase transitions) are closely linked to electronic structure changes induced by the presence of hydrogen. We are interested in examining the fundamental interaction of hydrogen and the metal lattice in this strongly coupled system. Most earlier theoretical studies were not self-consistent and very few considered the total energy of the system. Therefore a complete study is being carried using pseudopotential methods within the local-density approximation.

We started with the 4d transition metal series, with yttrium being the first element of interest. The structural properties were studied first to test the theoretical approach, in which we determined the energy cutoff for the basis set, the effect of different exchange-correlation energy functionals, and a correction for core-valence charge overlap. Then we studied the solid-solution phase with hydrogen occupying the tetrahedral sites. There have been speculations that the formation of pairs of hydrogen are responsible for a certain resistivity anomaly and the lack of precipitation down to very low temperature. In our calculation, we provided the first reliable estimate of the pairing energy and geometry. In addition, the classical potential surface, local vibrational modes and diffusion paths have been studied. The results are being written up.

For the high-concentration dihydride and trihydride phases, we studied the change of bonding characteristics and the structural transformation of the metal lattice. An interesting

new finding is that, because of the strong correlation between the hydrogen position and the electronic structure of the system, a so-called Peierls distortion gives rise to a semimetal-semiconductor transition and a frozen-in hydrogen vibrational wave in the metal lattice of the trihydride. More detailed analysis will be conducted in the next year.

Future works planned on this topic include the study of order-disorder transitions in the YH_{2+x} phase and investigations of the hydrogen-niobium and hydrogen-palladium systems which have very different metal lattices.

b. Tight-Binding Model for Elemental Semiconductors and Their Surfaces

To first order, the binding of elemental semiconductors can be described by their sp^3 orbitals. On the other hand, the distance and environmental dependence of the overlap integrals for these orbitals has not been examined closely in the past. Most previous calculations simply assumed a not-well-justified functional form. We have carefully determined these parameters by fitting the energy dispersions and total energy curves obtained from first-principles calculations. With these transferable parameters, we are studying the effect of strain on the surface reconstruction of Ge(111), where an interesting surface structural transition is observed during the epitaxial growth.

c. Calculation of Phonon Spectra

The energy dispersion of phonons (elementary excitations of lattice vibrations in solids) as a function of wave vector has been an important input to the studies of various physical properties, such as heat capacities, thermal expansion coefficients, electron-phonon interaction matrices, superconducting transition temperatures, etc. Previously, the full spetrum has been obtained only from model fitting, or from computation of the linear response functions (limited to semiconductors). *Ab initio* calculations have been performed only for isolated symmetry points and along symmetry lines. We are proposing a method to project the real-space force constant matrix along d independent symmetry directions, where d is the dimensionality of the system. Then, by a limited number of supercell calculations of the planar force constants, the full force constant matrix can be reconstructed. The dynamical matrix at any arbitrary wave vector then can be determined and the full phonon spectra can be obtained completely from first principles for both metals and semiconductors.

d. Pseudopotential Method in Electronic-Structure Studies

The pseudopotential approximation is used in electronic-structure calculations to eliminate the need to account explicitly for core electrons. In general, the accuracy of this method can be improved by increasing the number of so-called reference energies. Unfortunately, in the current scheme the nonlocal potential operator becomes non-Hermitian when the number of reference energy is more than one and one is forced to adopt a generalized eigenvalue formalism. In this study I proposed a scheme to construct a Hermitian nonlocal potential with the scattering properties matched directly to the all-electron results as

closely as possible. Although it is an approximate operator, the transferability can be improved systematically in the construction. This will greatly simplify the nonlocal operations in large-scale computations.

PUBLICATIONS

"Pseudopotential Plane-Wave Calculation of the Structural Properties of Yttrium", Y. Wang and M. Y. Chou, Phys. Rev. **B 44**, 10339 (1991).

"Reformulation of Generalized Separable Pseudopotentials", M. Y. Chou, Phys. Rev. **B 45** (1992).

"*Ab initio* Calculation of Force Constants and Full Phonon Dispersions", S. Wei and M. Y. Chou, submitted to Phys. Rev. Lett.

"Asymmetric Phase Diagram and Coverage Dependent Interactions of Hydrogen on Metal Surfaces", S. N. Sun and M. Y. Chou, submitted to Surf. Sci.

G41-625

DMR-9157537

ANNUAL PROGRESS REPORT
(10/1/92 - 9/30/93)

May, 1993

M. Y. Chou
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SUMMARY OF RESEARCH

The objectives of my research are to investigate the electronic structure of condensed matter and to study its effects on the structural and dynamical properties of materials. The purpose of these studies is to provide unambiguous explanations for various interesting phenomena observed experimentally and to make reliable predictions of new materials properties from microscopic quantum theories.

a. Tight-Binding Model for Elemental Semiconductors and Their Surfaces

To first order, the binding of elemental semiconductors can be described by their sp^3 orbitals. On the other hand, the distance and environmental dependence of the overlap integrals for these orbitals has not been examined closely in the past. Most previous calculations simply assumed a not-well-justified functional form. We have carefully determined these parameters by fitting to the energy dispersions and total energy curves obtained from first-principles calculations. With these transferable parameters, we have studied the effect of strain on the surface reconstruction of Ge(111), where an interesting surface structural transition was observed during the epitaxial growth. The driving force and energy contributions from atoms with different geometry were analyzed.

b. Hydrogen in Transition Metals

Hydrogen is the smallest and lightest interstitial impurity in transition metals. It interacts strongly with the metal host and behaves like a three-dimensional lattice gas with extremely high mobility. The diversity of phenomena exhibited by these systems (such as structural, order-disorder, and metal-semiconductor phase transitions) are closely linked to the electronic structure changes induced by the presence of hydrogen. We are interested in examining the fundamental interaction of hydrogen and the metal lattice in this strongly coupled system. Most earlier theoretical studies were not self-consistent and very few considered the total energy of the system. Therefore a complete study has been carried out using the pseudopotential method within the local-density approximation.

We have studied the solid solution phase of hydrogen in hexagonal close-packed yttrium with a plane wave basis. The binding energies associated with different interstitial sites were evaluated and the occupation of the tetrahedral site was found to be energetically

favorable. The vibrational frequency and the diffusion barrier were in excellent agreement with experiment. In addition, the intriguing pairing phenomenon was investigated by calculating the total energy for various pairing configurations. It was found that the pairing of hydrogen across a metal atom was indeed energetically favorable compared with other pairs considered. The pairing was found to be closely connected with the electronic structure of the system.

The structural and electronic properties of YH_3 were also studied. It was found that the change of the hydrogen positions in the metal lattice had a significant effect in the system properties. The calculation confirmed that hexagonal YH_3 with the unusual wave-like hydrogen displacements was energetically more stable than the cubic structure. These hydrogen displacements were found to be Peierls-like distortions and associated with the charge density wave in this three-dimensional system. The possible existence of an excitonic insulating ground state was speculated based on the unusual electronic structure in this system.

PUBLICATIONS

S. Wei and M. Y. Chou, "Ab initio Calculation of Force Constants and Full Phonon Dispersions", Phys. Rev. Lett. **69**, 2799 (1992).

J. L. Mercer, Jr. and M. Y. Chou, "Tight-binding Total Energy Models for Silicon and Germanium", Phys. Rev. B **47**, 9366(1993).

S. N. Sun and M. Y. Chou, "Asymmetric Phase Diagram and Coverage Dependent Effective Pair Interactions for Hydrogen on Close-packed Metal Surfaces", Surf. Sci. **280**, 415 (1993).

J. L. Mercer, Jr. and M. Y. Chou, "Energetics of Si(111) and Ge(111) and the Effect of Strain", Phys. Rev. B **48** (in press).

M. Y. Chou, S. Wei, and D. Vanderbilt, "Comment on 'Should all Surfaces be Reconstructed?'", Phys. Rev. Lett. **70** (in press).

Y. Wang and M. Y. Chou, "Theoretical Study of the Binding Properties and Electronic Structure of Hydrogen in Yttrium", Z. Phys. Chem. (in press).

Y. Wang and M. Y. Chou, "Charge Density Waves in Hexagonal YH_3", submitted to Phys. Rev. Lett.

Y. H. Chen and M. Y. Chou, "A Continuous Feedback Approach in Controlling Chaos", submitted to Phys. Rev. Lett.

Y. Wang and M. Y. Chou, "Structural and Electronic Properties of Yttrium Trihydrides", submitted to Phys. Rev. B.

G-41-625
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DMR-9157537

ANNUAL PROGRESS REPORT
(10/1/93 - 9/30/94)

May 1994

M. Y. Chou
School of Physics
Georgia Institute of Technology
Atlanta, GA 30332

SUMMARY OF RESEARCH

a. Tight-Binding Model for Elemental Semiconductors and Their Surfaces

We have carefully determined the tight-binding parameters for silicon and germanium by fitting to energy dispersions and total energy curves obtained from local-density calculations. With these transferable parameters, we have studied the effect of strain on the surface reconstruction of Ge(111), where an interesting surface structural transition was observed during the epitaxial growth. The driving force of the reconstruction and energy contributions from atoms of different geometry were analyzed. It was also found that by including two-center intra-atomic parameters, the structure-dependent term in the total energy model can be effectively eliminated.

b. Hydrogen in Transition Metals

We have studied the solid solution phase of hydrogen in hexagonal close-packed yttrium by first-principles calculations. The intriguing pairing phenomenon was investigated by calculating the total energy for various pairing configurations. It was found that the pairing of hydrogen across a metal atom was indeed energetically favorable compared with other pairs considered. The pairing was found to be closely connected with the electronic structure of the system.

The phase stability for beta-phase YH_{2+x} was investigated by the cluster variational method with the effective interactions obtained from first-principles total energy data. The calculated order-disorder transition temperature was consistent with the recent observation of the metal-semiconductor transition and resistivity anomalies near the same temperature range.

The structural and electronic properties of YH_3 were also studied. It was found that the change of hydrogen positions in the metal lattice had a significant effect in the system properties. The calculation confirmed that hexagonal YH_3 with the unusual wave-like hydrogen displacements was energetically more stable than the cubic structure. These hydrogen displacements were found to be Peierls-like distortions and associated with the charge density wave in this three-dimensional system. The possible existence of an excitonic insulating ground state was speculated based on the unusual electronic structure in this system.

c. Thermodynamic Properties of Silicon

We have performed a fully ab initio calculation of the thermodynamic properties for silicon within the quasiharmonic approximation, making use of volume-dependent phonon frequencies obtained from pseudopotential local-density calculations. The temperature dependence of the thermal expansion coefficient, specific heat, and other related quantities were studied. The abnormal (negative) thermal expansion coefficient at low temperatures was explained through a detailed study of mode Gruneisen parameters.

PUBLICATIONS

S. Wei and M. Y. Chou, "First-Principles Calculation of Force Constants and Full Phonon Dispersions", in "Materials Theory and Modelling" ed. by J. Broughton, P. Bristowe, and J. Newsam (Materials Research Society, Pittsburgh, 1993), p.641.

M. Y. Chou, S. Wei, and D. Vanderbilt, "Comment on 'Should all Surfaces be Reconstructed?'", Phys. Rev. Lett. **71**, 461 (1993).

J. L. Mercer, Jr. and M. Y. Chou, "Energetics of Si(111) and Ge(111) and the Effect of Strain'', Phys. Rev. B. **48**, 5374 (1993).

Y. Wang and M. Y. Chou, "Peierls Distortion in Hexagonal YH_3", Phys. Rev. Lett. **71**, 1226 (1993).

Y. Wang and M. Y. Chou, "Theoretical Study of the Binding Properties and Electronic Structure of Hydrogen in Yttrium", Z. Phys. Chem. Bd. **181**, S. 39 (1993)

S. N. Sun, Y. Wang, and M. Y. Chou, "First-Principles Study of Hydrogen Ordering in beta-YH_{2+x}", Phys. Rev. B. **49**, 6481 (1994).

J. L. Mercer, Jr. and M. Y. Chou, "Tight-Binding Model with Intra-Atomic Matrix Elements", Phys. Rev. B. **49**, 8506 (1994).

Y. Wang and M. Y. Chou, "Energetics and Lattice Contraction in beta-phase YH_{2+x}", Phys. Rev. B. **49**, 10731 (1994).

Y. Wang and M. Y. Chou, "Pseudopotential Total Energy Study of alpha-YH_x", Phys. Rev. B. **49** (in press).

S. Wei and M. Y. Chou, "Phonon Dispersions of Silicon and Germanium from First-Principles Calculations", Phys. Rev. B **50** (in press).

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CERTIFICATION PAGE

Certification for Principal Investigators and Co-Principal Investigators:

I certify to the best of my knowledge that:

(1) the statements herein (excluding scientific hypotheses and scientific opinions) are true and complete, and
(2) the text and graphics herein as well as any accompanying publications or other documents, unless otherwise indicated, are the original work of the signatories or individuals working under their supervision. I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this application.

I understand that the willful provision of false information or concealing a material fact in this proposal or any other communication submitted to NSF is a criminal offense (U.S.Code, Title 18, Section 1001).

Name (Typed)	Signature	Date
PI/PD MEI-YIN CHOU	Mei-Yin Chou	APRIL 15, 1995
Co-PI/PD		
Co-PI/PD		
Co-PI/PD		
Co-PI/PD		

Certification for Authorized Institutional Representative or Individual Applicant:

By signing and submitting this proposal, the individual applicant or the authorized official of the applicant institution is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding Federal debt statue, debarment and suspension, drugfree workplace, and lobbying activities (see below), as set forth in the Grant Proposal Guide (GPG), NSF 94-2. Willful provision of false information in this application and its supporting documents or in reports required under an ensuing award is a criminal offense (U.S. Code, Title 18, Section 1001).

Debt and Debarment Certifications

(If answer "yes" to either, please provide explanation.)

Is the organization delinquent on any Federal debt? Yes___ No X

Is the organization or its principals presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal department or agency? Yes___ No X

Certification Regarding Lobbying

This certification is required for an award of a Federal contract, grant, or cooperative agreement exceeding $100,000 and for an award of a Federal loan or a commitment providing for the United States to insure or guarantee a loan exceeding $150,000.

Certification for Contracts, Grants, Loans and Cooperative Agreements

The undersigned certifies, to the best of his or her knowledge and belief, that:

(1) No federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.

(2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure Form to Report Lobbying," in accordance with its instructions.

(3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by section 1352, title 31, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than $10,000 and not more than $100,000 for each such failure.

AUTHORIZED INSTITUTIONAL REPRESENTATIVE	SIGNATURE	DATE
NAME/TITLE (TYPED) DAVID B. BRIDGES / CONTRACTING OFFICER	David B. Bridges	4/19/95

TELEPHONE NUMBER	ELECTRONIC MAIL ADDRESS	FAX NUMBER
(404)894-4817	David.Bridges@OCA.GATECH.EDU	(404)894-6956

DMR-9157537

ANNUAL PROGRESS REPORT
(10/1/94 - 9/30/95)

April 1995

M. Y. Chou
School of Physics
Georgia Institute of Technology
Atlanta, GA 30332

SUMMARY OF RESEARCH

a. Hydrogen in Transition Metals

We have finished calculations on the structural and electronic properties of YH_3. It was found that the change of hydrogen positions in the metal lattice had a significant effect in the system's properties. The calculation confirmed that hexagonal YH_3 with the unusual wave-like hydrogen displacements was energetically more stable than the cubic structure. These hydrogen displacements were found to be Peierls-like distortions and associated with the charge density wave in this three-dimensional system. The possible existence of an excitonic insulating ground state was speculated based on the unusual electronic structure in this system.

b. Tight-Binding Model for Semiconductors

For many large systems that cannot be handled by first-principles studies, the semiempirical tight-binding method is a promising alternative. Before applying it with confidence, its accuracy has to be examined and, if possible, improved by comparing results with first-principles calculations and by including first-principles data in the fitting. We have reexamined the applicability of this approach in semiconductors by fitting two-center, orthogonal tight-binding parameters to LDA band structures in order to determine their distance dependence. It is also found that intra-atomic matrix elements, which were not included in previous tight-binding models, are quite important in describing the environmental change. After incorporating these parameters in the fitting and including a two-body potential to take into account the double counting in the band energy, reasonable total energies are obtained for many different bulk structures by a simple total energy model. Studies have been conducted for Si, Ge, C, and their alloys.

c. Hydrogen Adsorption on W(110)

Hydrogen adsorption on W(110) induces drastic changes in the structural and electronic properties of the surface, including a surface reconstruction, and a pronounced anomaly in the surface phonon spectra. Using the pseudopotential total-energy approach, we studied surface structures and electronic properties of clean and hydrogen-covered

W(110) surfaces. From the calculation we found that a surface reconstruction, consisting of a shift of the W top layer in the <1$\bar{1}$0> direction, is energetically favorable for the H-covered surface. We also found that adsorption of H induces one-dimensional Fermi-surface nesting in the $\bar{\Gamma}\bar{H}$ direction, which corresponds to exactly the same wave vector found in the surface-phonon anomaly along this direction. This result suggests that the phonon anomaly is a Kohn anomaly associated with Fermi-surface nesting. The possibility of Peierls distortion of hydrogen on the surface and of the formation of a charge-density wave, due to this electronic instability, is being investigated.

c. Wavelets in Electronic Structure Calculations

A wavelet basis consists of dilations and translations of a so-called "mother wavelet", and is a complete set for square integrable functions. It can be used to represent a function at different resolution levels, and to effectively describe rapid local variation. We have studied the feasibility of using these bases in solving the eigenvalue problem in electronic structure calculations. In particular, its efficiency in LDA self-consistent calculations have been carried out for several molecular systems.

PUBLICATIONS

J. L. Mercer, Jr. and M. Y. Chou, "Tight-Binding Model with Intra-Atomic Matrix Elements", Phys. Rev. B. **49**, 8506 (1994).

Y. Wang and M. Y. Chou, "Energetics and Lattice Contraction in beta-phase YH_{2+x}", Phys. Rev. B. **49**, 10731 (1994).

Y. Wang and M. Y. Chou, "Pseudopotential Total Energy Study of alpha-YH_x", Phys. Rev. B. **49**, 13357 (1994).

S. Wei and M. Y. Chou, "Phonon Dispersions of Silicon and Germanium from First-Principles Calculations", Phys. Rev. B **50**, 2221 (1994).

S. Wei and M. Y. Chou, "First-Principles Determination of Equilibrium Crystal Shapes for Metals at T = 0", Phys. Rev. B **50**, 4859 (1994).

Y. H. Chen and M. Y. Chou, "Continuous Feedback Approach for Controlling Chaos", Phys. Rev. E **50**, 2331 (1994).

S. Wei, C. Li, and M. Y. Chou, "Ab initio Calculation of Thermodynamic Properties", Phys. Rev. B **50**, 14587 (1994).

Y. Wang and M. Y. Chou, "Structural and Electronic Properties of Hexagonal Yttrium Trihydride", Phys. Rev. B **51** (in press).

SUMMARY PROPOSAL BUDGET

ORGANIZATION GEORGIA TECH RESEARCH CORPORATION				FOR NSF USE ONLY PROPOSAL NO.	DURATION (MONTHS) Proposed / Granted
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR MEI-YIN CHOU				AWARD NO.	

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By Proposer	Funds Granted By NSF (If Different)
1. MEI-YIN CHOU			1	$ 6,640	$
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (1) TOTAL SENIOR PERSONNEL (1-6)				6,640	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	11				27,338
2. ( ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)					
3. (1) GRADUATE STUDENTS				14,447	
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				21,087	27,338
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS) 24.7% of A1+B1				1,640	6,753
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				22,727	34,091
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $1,000.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
F. PARTICIPANT SUPPORT COSTS 1. STIPENDS $ 2. TRAVEL 3. SUBSISTENCE 4. OTHER					
( ) TOTAL PARTICIPANT COSTS					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					
H. TOTAL DIRECT COSTS (A THROUGH G)				22,727	34,091
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 10% of H					
TOTAL INDIRECT COSTS				2,273	3,409
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)					
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPM 252 AND 253)					
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ 25,000	$ 37,500

M. COST SHARING: PROPOSED LEVEL $	AGREED LEVEL IF DIFFERENT $			
PI/PD TYPED NAME & SIGNATURE* MEI-YIN CHOU Mei-Yin Chou	DATE 4/15/95	FOR NSF USE ONLY INDIRECT COST RATE VERIFICATION		
INST. REP. TYPED NAME & SIGNATURE* DAVID B. BRIDGES David B. Bridges	DATE 4/18/95	Date Checked	Date of Rate Sheet	Initials-ORG

NSF Form 1030 (1/94) *Supersedes All Previous Editions*

*SIGNATURES REQUIRED ONLY FOR REVISED BUDGET (GPM 233)

OMB 3145-0058

NATIONAL SCIENCE FOUNDATION
PRESIDENTIAL YOUNG INVESTIGATOR AWARDS PROGRAM
REQUEST FOR BASE AND/OR MATCHING FUNDS

PYI NAME: Mei-Yin Chou **DATE of REQUEST** April 15, 1995

NSF AWARD # DMR-9157537 **YEAR OF PYI AWARD** 1991

DESCRIPTION OF REQUESTS

	YES	NO (CHECK)	YEAR OF REQUESTS (CIRCLE)	AMOUNTS CASH	AMOUNTS EQUIPMENT
NSF BASE	X		1 2 3 4 5	$25,000	
MATCHING	X		1 2 3 4 5	$37,500	

DATE RESEARCH ACTIVITY INITIATED 10/1/91

MATCHABLE SOURCES (LISTED INDIVIDUALLY)	ADDRESS	CODE*	CASH	EQUIPMENT
1. The David and Lucile Packard Foundation	300 Second Street, Suite 200 Los Altos, CA 94022 (415) 948-7658	E21	$100,000	
2.				
3.				
4.				

NOTES:
- The NSF base award is $25,000; the maximum amount of matching funds is $37,500 for each activity year.
  Research activity must start by October 1, of award year. The awardee must designate starting date for research activity.

SOURCE CODES*

NON-PROFIT
- E21 Private Non-Profit (e.g. foundations)
- Business
- E22 State government
- E23 Local government

PROFIT
- F30 Large Corp. or
- F31 Small Corp. or Business
- H50 US Citizen or Resident
- I64 Foreign Organization

G-41-625
#5

DMR-9157537

ANNUAL PROGRESS REPORT
(10/1/95 - 9/30/96)

May 1996

M. Y. Chou
School of Physics
Georgia Institute of Technology
Atlanta, GA 30332

SUMMARY OF RESEARCH

a. Hydrogen in Transition Metals

We have studied total energies of various ordered structures of PdH_x (in which hydrogen occupies the octahedral sites within the fcc Pd lattice). For x larger than 0.5, we found that the NiMo- and Ni_4Mo-type structures at x=0.5 and 0.8, respectively, were energetically favored phases, in agreement with the superlattice reflections found in previous neutron-scattering measurements. For intermediate concentrations, linear variation of the formation energy as a function of x in several (420)-ordered structures explained the observed short-range order. We also finished the study on YH_3 and had the final paper published. The calculation confirmed that hexagonal YH_3 with the unusual wave-like hydrogen displacements was energetically more stable than the cubic structure. These hydrogen displacements were found to be Peierls-like distortions and associated with the charge density wave in this three-dimensional system.

b. Hydrogen Adsorption on W(110)

Hydrogen adsorption on W(110) induces drastic changes in the structural and electronic properties of the surface, including a surface reconstruction, and a pronounced anomaly in the surface phonon spectra. Using the pseudopotential total-energy approach, we studied surface structures and electronic properties of clean and hydrogen-covered W(110) surfaces. From the calculation we found that a surface reconstruction, consisting of a shift of the W top layer in the <110> direction, is energetically favorable for the H-covered surface. The first paper has been published in the Physical Review B. We also found that adsorption of H induces hidden one-dimensional Fermi-surface nesting in the same fashion as found in the two-dimensional charge-density-wave compounds. This result suggests that the phonon anomaly is a Kohn anomaly associated with Fermi-surface nesting. The possibility of Peierls distortion of hydrogen on the surface and of the formation of a charge-density wave, due to this electronic instability, is being studied.

c. Wavelets in Electronic Structure Calculations

A wavelet basis consists of dilations and translations of a so-called "mother

wavelet", and is a complete set for square integrable functions. It can be used to represent a function at different resolution levels, and to effectively describe rapid local variation. We have studied the feasibility of using these bases in solving the eigenvalue problem in electronic structure calculations. In particular, its efficiency in LDA self-consistent calculations have been carried out for several molecular systems. The work has been published in Physical Review Letters.

PUBLICATIONS

Y. Wang and M. Y. Chou, "Structural and Electronic Properties of Hexagonal Yttrium Trihydride", Phys. Rev. B **51**, 7500 (1995).

M. Y. Chou, "Shell Structure in Metal Clusters", in Quantum Theory of Real Materials, edited by J. R. Chelikowsky and S. G. Louie (Kluwer, 1996).

Y. Wang and M. Y. Chou, "Total-Energy Study of Hydrogen Ordering in PdH_x ($0<x<1$)", Phys. Rev. B **53**, 1 (1996).

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ANNUAL PROGRESS REPORT
(10/1/96 - 9/30/97)

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SUMMARY OF RESEARCH

a. **Hydrogen on Semiconductor Surfaces**

Hydrogen is a common impurity that plays an important role in semiconductor growth. It affects the stability of different phases on the surface in a significant way. We have evaluated the surface free energies of hydrogen-covered (100), (111), and (110) surfaces of diamond and silicon as a function of hydrogen chemical potential using first-principles pseudopotential methods. The change in surface energy anisotropy and equilibrium crystal shape due to hydrogen adsorption is carefully examined. The three low-index facets are affected differently by the presence of hydrogen and unexpected differences are found between diamond and silicon. Taking into account possible formation of local facets on the hydrogen-covered (100) surfaces, we find that the dihydride phase is not stable on both C(100) and Si(100), nor is the 3x1 phase on C(100).

b. **Quantum Monte Carlo Study of Electron Exchange and Correlation in Silicon**

A combination of the coupling constant integration technique and the quantum Monte Carlo method is used to investigate the most relevant quantities in Kohn-Sham density functional theory. The variational quantum Monte Carlo method is used to construct realistic many-body wave functions for diamond-structure silicon at different values of the Coulomb coupling constant. The exchange-correlation energy density along with the coupling constant dependence and the coupling-constant-integrated form of the pair correlation function, the exchange-correlation hole, and the exchange-correlation energy are calculated. The pair correlation function is found to have a correlation contribution which is more localized and isotropic than its exchange counterpart. With increasing Coulomb repulsion, the electron "digs" out a deeper correlation hole that exhibits a longer range. We also compared these functions with results obtained from the local density approximation, the average density approximation, the weighted density approximation, and the generalized gradient approximation. The success of the local density approximation can be viewed as a result of several errors which cancel in the evaluation of the total exchange-correlation energy, including a real-space cancellation that has not been discovered in the past.

PUBLICATIONS

A. J. Williamson, G. Rajagopal, R. J. Needs, L. M. Fraser, W. M. C. Foulkes, Y. Wang, and M. Y. Chou, "Elimination of Coulomb Finite Size Effect in Quantum Many-Body Simulations", Phys. Rev. B **55**, R4851 (1997).

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#7

FINAL REPORT FOR AWARD # 9157537

Mei-Yin Chou ; *GA Tech Res Corp - GIT*
Presidential Young Investigator Award

Participant individuals:
Post-doc(s): Sheng N Sun; Siqing Wei; Kook-Whee Kwak; Suklyun Hong; Randolph Q Hood; Antonio Cancio
Graduate student(s): Yan Wang; Changlin Li; Aaron Puzder

Participants' Detail

Partner organizations:
Other collaborators:

J.J. Rush's group at NIST and Richard Needs at Cambridge University.

Activities and findings:

Research Activities:

The objectives of my project are to investigate the electronic structure of condensed matter and to study its effects on the structural and dynamical properties of materials. For systems with translational symmetry, calculations are performed from first principles with no adjustable parameters. This has been made possible by advances in computational methods developed in the past decades. When these first-principles calculations are not feasible in some larger and more complicated systems, model calculations are used to identify the important features. The purpose of these studies is to provide unambiguous explanations for various interesting phenomena observed experimentally in solids and surfaces, and to make reliable predictions of new material properties from microscopic quantum theories.

Our theoretical efforts can be classified into two categories: (1) the study of the electronic and dynamical properties of technologically important materials, and (2) the development of new algorithms and calculational methods in studying materials properties using quantum mechanics.

Activities and findings:

Research Findings:

(1) Hydrogen in Metals

Hydrogen is the smallest and lightest interstitial impurity in transition metals. It interacts strongly with the metal host and behaves like a three-dimensional lattice gas with extremely high mobility. The diversity of phenomena exhibited by these systems (such as structural, order-disorder, and metal-semiconductor phase