Final Project Report of UGC Major Research Project for the period 01/04/2013 to 30/11/2016)

"Vibrational Response and Phase transition in certain non-simple metals and alloys covering wide range of densities"

F. No. 42-771\ 2013 (SR)
Dated: 14-3-2013

By

Dr. N. K. Bhatt
Department of Physics
Sardar Patel University
Vallabh Vidyanagar – 388 120
Gujarat, India

Annexure – III

STATEMENT OF THE EXPENDITURE IN RESPECT OF MAJOR RESEARCH PROJECT

1. Name of Principal Investigator : **Dr. N. K. Bhatt**

2. Dept. of University/ College : Department of Physics,
   Sardar Patel University,
   Vallabh Vidyanagar. 388 120

3. UGC approval Letter No. and Date : **F. No. 42-771\ 2013 (SR) dated on 01-04-2013**

4. Title of the Research Project : "Vibrational Response and Phase transition in certain non-simple metals and alloys covering wide range of densities"

5. Effective date of starting the project : **1st April 2013**

6. (a) Period of Expenditure : From **01/04/2013 to 31/03/2014 (Ist term)**
   01/04/2014 to 31/03/2015 (IInd term)
   01/04/2015 to 31/03/2016 (IIIrd term)
   01/04/2016 to 30/11/2016 (IVth term)

(b) Details of Expenditure:

Sr. No.	Item	Amount Approved (Rs.)	Expenditure Incurred (Rs.)				
			01/04/2013 to 31/03/2014 (1st term)	01/04/2014 to 31/03/2015 (IInd term)	01/04/2015 to 01/04/2016 (IIIrd term)	01/04/2016 to 01/11/2016 (IIIrd term)	Total
i	Book & Journals	30,000/-	0	0	29,433/-	0	29,433/-
ii	Equipment	3,00,000/-	50,000/-	1,18,657/-	1,31,343/-	---	3,00,000/-
iii	Contingency	60,000/-	14,280/-	12,160/-	25,201/-	5870/-	57,511/-
iv	Field Work/ Travel (Give details in the proforma at Annexure-IV).	---	---	---	---	----	---
v	Hiring Services	---	---	---	---	---	---
vi	Chemicals & Glassware	---	---	----	----	---	----
vii	Overhead	58,800/-	58,800/-	---	---	---	58,800/-
vii	Any other items (Please specify)	---	---	---	----	---	---
	Total	**4,48,800/-**	**1,23,080/-**	**1,30,817/-**	**1,85,977/-**	**5,870/-**	**4,45,744/-**

c. Staff : **Ms. Rajani H. Joshi (Project fellow)**
Date of Appointment : **1st August 2013**

S. No.	Items	From	To	Amount Approved (Rs.)	Expenditure incurred (Rs.)
1	Project Fellow @Rs. 14,000/-p.m.	1st August 2013	31st 2014	5,28,000/-	98,000/-
2	Project Fellow @Rs. 14,000/-p.m.	1st April 2014	31st March 2014		1,68,000/-
3	Project Fellow @Rs. 14,000/-p.m. till August – 2015 and @Rs. 16,000/- till March	1st April 2015	31st July 2016		2,62,000/-
	Total				**5,28,000/-**
	H.R.A			52,800/-	**52,800/-**
	Total				**5,80,800/-**

1. It is certified that the appointment(s) have been made in accordance with the terms and conditions laid down by the Commission.

2. If as a result of check or audit objection some irregularly is noticed at later date, action will be taken to refund, adjust or regularize the objected amounts.

3. Payment @ revised rates shall be made with arrears on the availability of additional funds.

4. It is certified that the grant of **Rs.6,82,800/-(Rupees Seven lakh ninety thousand three hundred only) (1st installment)+ Rs.2,82,720/-(Rupees Two lakh eighty two thousand seven hundred twenty only) (2nd installment)** has been received from the University Grants Commission under the scheme of support for Major Research Project entitled **"Vibrational Response and Phase transition in certain non-simple metals and alloys covering wide range of densities" vide UGC letter No. F. No. 42-771/2013 (SR) dated 31nd March, 2013. Out of this Rs. 2,21,080/- (Rupees Two lakhs twenty one thousand eighty only) (1st term) +Rs. 2,98,817/- (Rupess Two lakhs fifty Six thousand eight hundred seventeen only) (IInd term) + Rs. 3,83,977/- (Rupess Three lakhs eighty three thousand nine hundred seventy seven only) (IIIrd term) + Rs. 1,22,670/- (Rupess one lakh twenty two thousand six hundred seventy only) (IVth term) = Total Rs. 10,26,544/-**has been utilized for the purpose for which it was sanctioned and in accordance with the terms and conditions laid down by the University Grants Commission.

SIGNATURE OF THE PRINCIPAL INVESTIGATOR (Dr. N. K. Bhatt) **REGISTRAR**

SIGNATURE OF THE CO-INVESTIGATOR
(Dr. A. R. Jani)

Annexure – VII

MAJOR RESEARCH PROJECT HOUSE RENT FOR PROJECT FELLOW

Certified that Ms.Rajani H. Joshi is paying House Rent of Rs.1400/- and is eligible to draw House Rent Allowances @10% **1400 *24 + 1600*12= 52,800/-** as per University Rules.

SIGNATURE OF THE PRINCIPAL INVESTIGATOR (Dr. N. K. Bhatt)

REGISTRAR

SIGNATURE OF THE CO-INVESTIGATOR
(Dr. A. R. Jani)

STATEMENT OF THE HOUSE RENT IN RESPECT OF MAJOR RESEARCH PROJECT

Sr No.	Month	How much to be reimburse
1.	August 2013	1400/-
2.	September 2013	1400/-
3.	October 2013	1400/-
4.	November 2013	1400/-
5.	December 2013	1400/-
6.	January 2014	1400/-
7.	February 2014	1400/-
8.	March 2014	1400/-
9.	April 2014	1400/-
10.	May 2014	1400/-
11.	June 2014	1400/-
12.	July 2014	1400/-
13.	August 2014	1400/-
14.	September 2014	1400/-
15.	October 2014	1400/-
16.	November 2014	1400/-
17.	December 2014	1400/-
18.	January 2015	1400/-
19.	February 2015	1400/-
20.	March 2015	1400/-
21.	April 2015	1400/-
22.	May 2015	1400/-
23.	June 2015	1400/-
24.	July 2015	1400/-
25.	August 2015	1600/-
26.	September 2015	1600/-
27.	October 2015	1600/-
28.	November 2015	1600/-
29.	December2015	1600/-
30.	January 2016	1600/-
31.	February 2016	1600/-
32.	March 2016	1600/-
33.	April 2016	1600/-
34.	May 2016	1600/-
35.	June 2016	1600/-
36.	July 2016	1600/-
		TOTAL -52,800 /-

Annexure –VIII

Final Report of the work done on the Major Research Project

1. Project report No. : **Final Project Report**
2. UGC Reference No. : **F. No. 42-771\ 2013 (SR)**
3. Period of report : **From 01/04/2013 to 31/03/2014 (Ist term)**
   01/04/2014 to 31/03/2015 (IInd term)
   01/04/2015 to 31/03/2016 (IIIrd term)
   01/04/2016 to 30/11/2016 (IVth term)

4. Title of research project : **"Vibrational Response and Phase transition in certain non-simple metals and alloys covering wide range of densities"**

5. (a) Name of the Principle Investigator: **Dr. N. K. Bhatt**

   (b) Department. **Department of Physics**

   (c) University/College where work has progressed: **Department of Physics, Sardar Patel University, Vallabh Vidyanagar- 388 120 Gujarat**

6. Effective date of starting of project : **1st April 2013**

7. Grant approved and expenditure incurred during the period of the report:

   (a) Total amount approved: **Rs. 9,76,800/- + Rs. 52,800/- (HRA) = 10,29,600/-**

   Total amount Released: **Rs. 9,65,520/-**

   (b) Total expenditure: **Rs. 10,26,544/-**

   (c) Report of the work done: (Separate sheet attached)

   i. Brief objective of the project

   ii. Work done so far and results achieved and publications, if any, resulting from the work (Give details of the papers and names of the journals in which it has been published or accepted for publication……

REPORT OF THE WORK DONE

(A) TITLE OF THE PROJECT:

"Vibrational Response and Phase Transition in Certain Non-Simple Metals and Alloys Covering Wide Range of Densities"

(B) BRIEF OBJECTIVE OF THE PROJECT:

The main objective of this project is to investigate, if possible, a uniform approach of calculating several physical properties covering wide range of density. Historically there appears two distinct approaches to study high-density solid state phase and low density fluid state. In order to fulfill this task, we have concentrated on the compressed state of matter (high-density state) for elemental metals Ir, Na, W, Ta and also compounds like NbC, GaP, CaS, and Na_2O. These results were presented and published at conferences and in journals. Currently, we are concentrating to calculate thermal properties for Copper, Silver, Gold and Aluminum using first principles density functional quasiharmonic approximation in conjunction with empirical but true anharmonic contribution. This newly proposed accurate scheme (so-called semi first-principles) capable of capturing all anharmonic effects in physical properties is used to compute properties along shock Hugoniot. For fluid phase we have proposed and used model pseudopotential to calculate atomic properties of Copper, Silver, Gold and Aluminium.

(C) WORK DONE:

- In order to calculate thermophysical properties of non-simple metals such as noble metals at higher temperatures and pressures we have coupled first principles calculations to various other models.

- In order to compute the vibrational properties of non-simple metals and alloys, we have employed Quantum espresso code. Phonon-dispersion curve (pdc) and phonon density-of-state (p-dos) were computed through DFPT using QE-code, while volume dependence of phonon frequency were calculated through mode Grüneisen parameter by using numerical differentiation. Based on an assumption of linear dependence of the phonon frequency on volume, we could calculate pdc at different compressed volume or equivalent densities.

- For electrons we have taken another other model, as from the literature we understood that, on expanding the Thomas Fermi expression for electron energy at very low temperature and keeping the terms up to T2 one obtains with the theoretical b0. Even if one replaces this theoretical estimate of b0 with its experimental value, the question whether the temperature is sufficiently low for such expansion remains debatable. Both the facts cause TF theory to estimate the electron pressure incorrectly. McCloskey (1964) formula seems to be a better choice, as it finds the energy and pressure for any temperature by using proper fitting constants. This approach provides the correct electron pressure and energy upto about two to three times the critical temperature.

- For calculating intrinsic anharmonicity leads to temperature dependence of phonon frequency. Over and above these phonon-anharmonicity; thermally excited electrons also have deceive role and contribute significantly close to melting temperature.

- Various high pressure properties has been calculated and for that a new approach for the calculation of Grüneisen parameter has chosen and many important properties like shock Hugoniot Pressure and Temperature, Melting Curve and various thermodynamical properties along Shock Hugoniot has been calculated.

- For liquid state, new model pseudopotential has been given to calculate various atomic properties have been calculated. Even the transferability of the pseudopotential from solid to liquid state has been checked.

- In order to calculated various above mentioned properties at varying densities various computing facilities has been used and various books and other consumables was needed , hence full grant has been procured.

- One M.Phil student and one Ph.d student has been trained during this project.

- Results obtained from the calculations have been presented in various conferences, seminar, symposia and has been published in various journal are encouraging which will be shortly published in journals of international repute.

Having all these we generated some important results that has been presented in some of the below conferences:

Paper Published

1) **Lattice Dynamics of fcc-Iridium**
   R. H. Joshi, A. Y. Vahora, A. B. Patel, N. K. Bhatt, B. Y. Thakore, and A. R. Jani
   Quantum Matter, Vol. 5, 1–3, 2016

2) **Atomic Transport In Liquid Aluminum Using a New Pseudopotential**
   R. H. Joshi, D. D. Satikunvar, N. K. Bhatt, B. Y. Thakore and A. R. Jani
   Advanced Materials Research, Online: 2016-08-22 ISSN: 1662-8985, Vol. 1141, pp 24-28 doi:10.4028/www.scientific.net/AMR.1141.24

3) **Theoretical Modeling of Equations of States for Aluminum to Pressure up to 10 TPa and Temperature to 10 eV**
   N. K. Bhatt, R. H. Joshi, B. Y. Thakore, A. R. Jani and P. R. Vyas
   Advanced Materials Research Online: 2016-08-22, ISSN: 1662-8985, Vol. 1141, pp 121-124 doi:10.4028/www.scientific.net/AMR.1141.121

4) **High-temperature thermodynamics of silver: Semi–empirical approach**
   R. H. Joshi , B Y Thakore , P R Vyas , A R Jani , and N K Bhatt
   Chinese Physics B, Vol. 26, No. 11, 116502, 2017.

5) **Semi-empirical anzatz for Helmholtz free energy calculation: Thermal properties of silver along shock Hugoniot**
   R. H. Joshi, B. Y. Thakore, N. K. Bhatt, P. R. Vyas, A. R. Jani
   Physica B: Condensed Matter, 530, 1 February 2018, Pages 160-166

6) **Grüneisen parameter and equations of states for copper–High pressure study**
   R. H. Joshi, B. Y. Thakore, N. K. Bhatt, P. R. Vyas, A. R. Jani
   Computational Condensed Matter,15, June 2018, Pages 79-84

Paper Published in conference proceedings/paper presented in conferences:

1) Shock Hugoniot and High Pressure Melting Curve for NbC
   R. H. Joshi, A. Y. Vahora, N. K. Bhatt, B. Y. Thakore and A. R. Jani
   Proceedings of national Conference on Emerging Trends in Engineering, Technology and Management with the ISBN: 978-81-923049-9-1(Awarded best paper)

2) Pressure driven instability in Sodium
   P. R. Vyas, N. K. Bhatt , R. H. Joshi

Proceedings of national Conference on Emerging Trends in Engineering, Technology and Management with the ISBN: 978-81-923049-9-1

3) Equation of state for Tungsten: Shock Hugoniot
R. H. Joshi, N. K. Bhatt, B. Y. Thakore
UGC Sponsored One Day Seminar on Condensed Matter Physics (CMP-2014), 3rd March 2014. Organized by Department of Physics, Sardar Patel University, Vallabh Vidyanagar, Gujarat

4) Thermophysical properties of Calcium chalcogenides
R. H. Joshi, N. K. Bhatt and B. Y. Thakore
"National Seminar on Crystallography (NSC 43B) and National Workshop on CADD" organized by Department of Physics, Sardar Patel University, Vallabh Vidyanagar, Gujarat (01 – 03 September, 2014).

5) Lattice Dynamics and Thermophysical Properties of Na_2O at High Temperature
R. H. Joshi, D. D. Satikunvar, N. K. Bhatt, B. Y. Thakore and A. R. Jani
National conference Organized by University Grants Commission on "Recent Advances in Materials Science and Technology" held December 22-23, 2014 at Sh. M.L.V. Govt. College, Bhilwara (Rajasthan), ISBN: 978-81-930586-0-2.

6) A First Principles Phonon Dynamics of Cubic Boron Nitride
National conference Organized by University Grants Commission on "Latest Developments in Basic and Applied Sciences"
10th January 2015, M. B. Patel Science College, Anand (Gujarat)

7) Shock Equation of States of Au: A Mean-Field Potential Approach
National conference on condensed matter physics
27-28th March 2015 MIT University, Maniapal (Karnataka).

iii. Has the progress been according to original plan of work and towards achieving the objective? If not, state reasons: **YES**

iv. Please indicate the difficulties, if any, experienced in implementing the project: **No**

v. If project has not been completed, please indicate the approximate time by which it is likely to be completed. A summary of the work0 done for the period (Annual basis) may please be sent to the Commission on a separate sheet: **N.A.**

vi. If the project has been completed, please enclose a summary of the findings of the study. One bound copy of the final report of work done may also be sent to University Grants Commission: **Yes.**

vii. Any other information which would help in evaluation of work done on the project. At the completion of the project, the first report should indicate the output, such as (a) Manpower trained (b) Ph. D. awarded (c) Publication of results (d) other impact, if any.

a) 01 - M.phil degree awarded during this project.

b) 01 – Ph.d Synopsis Submitted.

c) Publications are discussed above.

SIGNATURE OF THE PRINCIPAL INVESTIGATOR (Dr. N. K. Bhatt)

REGISTRAR

SIGNATURE OF THE CO-INVESTIGATOR
(Dr. A. R. Jani)

Annexure – IX

PROFORMA FOR SUBMISSION OF INFORMATION AT THE TIME OF SENDING THE FINAL REPORT OF THE WORK DONE ON THE PROJECT

1. TITLE OF THE PROJECT: Vibrational Response and Phase transition in certain non-simple metals and alloys covering wide range of densities.

2. NAME AND ADDRESS OF THE PRINCIPAL INVESTIGATOR

Dr. N. K. Bhatt
Department of Physics
Sardar Patel University
Vallabh Vidyanagar – 388 120
Gujarat, India

3. NAME AND ADDRESS OF THE INSTITUTION

Department of Physics,
Sardar Patel University
Vallabh Vidyanagar – 388 120
Gujarat, India

4. UGC APPROVAL LETTER NO. AND DATE: F. No. 42-771\ 2013 (SR) Dated: 14-3-2013

5. DATE OF IMPLEMENTATION: 01-08-2013

6. TENURE OF THE PROJECT: 3 yrs + 01 extended by UGC.

7. TOTAL GRANT ALLOCATED: Rs. 9,76,800/- + Rs. 52,800/- (HRA) = 10,29,600/-

8. TOTAL GRANT RECEIVED: Rs. 9, 65,520/-

9. FINAL EXPENDITURE: Rs. 10, 26,544/-

10. TITLE OF THE PROJECT:

Vibrational Response and Phase transition in certain non-simple metals and alloys covering wide range of densities.

11. OBJECTIVES OF THE PROJECT:

- To study vibrational response of non-simple metals at high conditions, with focus on thermal properties.
- Presence of conduction electrons in metals, make their study important along strong shock Hugoniot conditions.
- High Pressure melting curve to explore solid-liquid phase boundary.
- Proposal of new local pseudopotential with its applications particularly, in its fluid phase.

12. WHETHER OBJECTIVES WERE ACHIEVED:

Yes, it was fully achieved abd briefly discussed in work done.

13. ACHIEVEMENTS FROM THE PROJECT:

- As per original proposal, uniform and consistent to address high Temperature and high pressure vibrational properties of non-simple metals, like Cu, Ag and Au is proposed.

- Solid-Liquid phase boundary under pressure is investigated.

- Atomic transport properties in the liquid phase have been computed employing our newly proposed pseudopotential.

14. SUMMARY OF THE FINDINGS:

- The Properties Studied in the Present Work are as Follows:

(i) Properties at high temperature:

- Cohesive energy as a function of volume.
- Phonon dispersion curve and phonon–density-of-state.
- Quasiharmonic Helmholtz free energy as a function of volume and temperature.
- Anharmonic total Helmholtz free energy as a function of volume and temperature.
- Linear thermal expansion coefficient.
- Isothermal bulk modulus.
- Adiabatic bulk modulus.
- Entropy.

- Enthalpy.
- Variation of specific heat at constant volume (C_V) with temperature.
- Variation of specific heat at constant pressure (C_P) with temperature.
- Temperature variation of thermodynamic Grüneisen parameter (γ_{th}).

(ii) Properties at high pressure:

- Pressure variation of thermodynamic Grüneisen parameter (γ_{th}).
- Static equation of state.
- Shock-Hugoniot (Dynamic) equation of state.
- Temperature along principal Hugoniot.
- Melting curve.
- Physical properties along Shock Hugoniot; viz. specific heat, enthalpy and Grüneisen parameter.

(iii) Liquid atomic transport properties:

- Comparison of form-factors.
- Inter-atomic pair-potential at different temperatures.
- Pair correlation function as a function of temperature.
- Variation of the dynamical structure factor at different wave vectors and as a function of temperature.
- The longitudinal current-current correlation function.
- Normalized velocity auto-correlation function.
- The self-diffusion coefficient as a function of temperature.
- Viscosity as a function of temperature.
- Cosine frequency power spectrum at different temperatures.
- Mean square displacement at different temperatures

15. CONTRIBUTION TO THE SOCIETY:

- From these Project 2 students has been guided and trained for their future work.
- The research which has been carried out will be helpful to the future researchers for extend their research further.

16. WHETHER ANY PH.D. ENROLLED/PRODUCED OUT OF THE PROJECT:

01 M.phil+ 01 Ph.d

17. NO. OF PUBLICATIONS OUT OF THE PROJECT: (ATTACHED)

SIGNATURE OF THE PRINCIPAL INVESTIGATOR (Dr. N. K. Bhatt) **REGISTRAR**

SIGNATURE OF THE CO-INVESTIGATOR
(Dr. A. R. Jani)

SUMMARY

"Vibrational Response and Phase transition in certain non-simple metals and alloys covering wide range of densities"

F. No. 42-771\ 2013 (SR)
Period 01/04/2013 to 30/11/2016

By

Dr. N. K. Bhatt
Department of Physics
Sardar Patel University
Vallabh Vidyanagar – 388 120
Gujarat, India

Total amount approved:	**Rs. 9,76,800/- + Rs. 52,800/- (HRA) = 10,29,600/-**
Total amount Released:	**Rs. 9,65,520/-**
Total expenditure:	**Rs. 10,26,544/-**

BRIEF OBJECTIVE OF THE PROJECT:

The main objective of this project is to investigate, if possible, a uniform approach of calculating several physical properties covering wide range of density. Historically there appears two distinct approaches to study high-density solid state phase and low density fluid state. In order to fulfill this task, we have concentrated on the compressed state of matter (high-density state) for elemental metals Ir, Na, W, Ta and also compounds like NbC, GaP, CaS, and Na_2O. These results were presented and published at conferences and in journals. Currently, we are concentrating to calculate thermal properties for Copper, Silver, Gold and Aluminum using first principles density functional quasiharmonic approximation in conjunction with empirical but true anharmonic contribution. This newly proposed accurate scheme (so-called semi first-principles) capable of capturing all anharmonic effects in physical properties is used to compute properties along shock Hugoniot. For fluid phase we have proposed and used model pseudopotential to calculate atomic properties of Copper, Silver, Gold and Aluminum.

WORK DONE:

- In order to calculate thermophysical properties of non-simple metals such as noble metals at higher temperatures and pressures we have coupled first principles calculations to various other models.

- In order to compute the vibrational properties of non-simple metals and alloys, we have employed Quantum espresso code. Phonon-dispersion curve (pdc) and phonon density-of-state (p-dos) were computed through DFPT using QE-code, while volume dependence of phonon frequency were calculated through mode Grüneisen parameter by using numerical differentiation. Based on an assumption of linear dependence of the phonon frequency on volume, we could calculate pdc at different compressed volume or equivalent densities.

- For electrons we have taken another other model, as from the literature we understood that, on expanding the Thomas Fermi expression for electron energy at very low temperature and keeping the terms up to T^2 one obtains with the theoretical b0. Even if one replaces this theoretical estimate of b0 with its experimental value, the question whether the temperature is sufficiently low for such expansion remains debatable. Both the facts cause TF theory to estimate the electron pressure incorrectly. McCloskey (1964) formula seems to be a better choice, as it finds the energy and pressure for any temperature by using proper fitting constants. This approach provides the correct electron pressure and energy upto about two to three times the critical temperature.

- For calculating intrinsic anharmonicity leads to temperature dependence of phonon frequency. Over and above these phonon-anharmonicity; thermally excited electrons also have deceive role and contribute significantly close to melting temperature.

- Various high pressure properties has been calculated and for that a new approach for the calculation of Grüneisen parameter has chosen and many important properties like shock Hugoniot Pressure and Temperature, Melting Curve and various thermodynamical properties along Shock Hugoniot has been calculated.

- For liquid state, new model pseudopotential has been given to calculate various atomic properties have been calculated. Even the transferability of the pseudopotential from solid to liquid state has been checked.

- In order to calculated various above mentioned properties at varying densities various computing facilities has been used and various books and other consumables was needed , hence full grant has been procured.

- One M.Phil. student and one Ph.D. student has been trained during this project.

- Results obtained from the calculations have been presented in various conferences, seminar, symposia and has been published in various journal are encouraging which will be shortly published in journals of international repute.

Based on the proposal and work done we have generated some important results that has been published in journals of International reputes and presented at conferences:

Journal Publications….

1) Lattice Dynamics of fcc-Iridium
R. H. Joshi, A. Y. Vahora, A. B. Patel, N. K. Bhatt, B. Y. Thakore, and A. R. Jani
Quantum Matter, Vol. 5, 1–3, 2016

2) Atomic Transport in Liquid Aluminum Using a New Pseudopotential
R. H. Joshi, D. D. Satikunvar, N. K. Bhatt, B. Y. Thakore and A. R. Jani
Advanced Materials Research, Online: 2016-08-22 ISSN: 1662-8985, Vol. 1141, pp 24-28.

3) Theoretical Modeling of Equations of States for Aluminum to Pressure up to 10 TPa and Temperature to 10 eV
N. K. Bhatt, R. H. Joshi, B. Y. Thakore, A. R. Jani and P. R. Vyas
Advanced Materials Research Online: 2016-08-22, ISSN: 1662-8985, Vol. 1141, pp 121-124.

4) High-temperature thermodynamics of silver: Semi–empirical approach
R. H. Joshi, B Y Thakore, P R Vyas, A R Jani, and N K Bhatt
Chinese Physics B, Vol. 26, No. 11, 116502, 2017.

5) Semi-empirical anzatz for Helmholtz free energy calculation: Thermal properties of silver along shock Hugoniot
R. H. Joshi, B. Y. Thakore, N. K. Bhatt, P. R. Vyas, A. R. Jani
Physica B: Condensed Matter, 530, 1 February 2018, Pages 160-166

6) Grüneisen parameter and equations of states for copper–High pressure study
R. H. Joshi, B. Y. Thakore, N. K. Bhatt, P. R. Vyas, A. R. Jani
Computational Condensed Matter,15, June 2018, Pages 79-84

Papers Published in conference proceedings/paper presented at conferences….

1) Shock Hugoniot and High Pressure Melting Curve for NbC
R. H. Joshi, A. Y. Vahora, N. K. Bhatt, B. Y. Thakore and A. R. Jani
Proceedings of national Conference on Emerging Trends in Engineering, Technology and Management with the ISBN: 978-81-923049-9-1 (**Awarded best paper**).

2) Pressure driven instability in Sodium
P. R. Vyas, N. K. Bhatt, R. H. Joshi
Proceedings of national Conference on Emerging Trends in Engineering, Technology and Management with the ISBN: 978-81-923049-9-1

3) Equation of state for Tungsten: Shock Hugoniot
R. H. Joshi, N. K. Bhatt, B. Y. Thakore
UGC Sponsored One Day Seminar on Condensed Matter Physics (CMP-2014), 3rd March 2014.
Organized by Department of Physics, Sardar Patel University, Vallabh Vidyanagar, Gujarat.

4) Thermophysical properties of Calcium chalcogenides
R. H. Joshi, N. K. Bhatt and B. Y. Thakore

"National Seminar on Crystallography (NSC 43B) and National Workshop on CADD" organized by Department of Physics, Sardar Patel University, Vallabh Vidyanagar, Gujarat (01–03 Sept., 2014).

5) Lattice Dynamics and Thermophysical Properties of Na_2O at High Temperature
R. H. Joshi, D. D. Satikunvar, N. K. Bhatt, B. Y. Thakore and A. R. Jani
National conference Organized by University Grants Commission on "Recent Advances in Materials Science and Technology" held December 22-23, 2014 at Sh. M.L.V. Govt. College, Bhilwara (Rajasthan), ISBN: 978-81-930586-0-2.

6) A First Principles Phonon Dynamics of Cubic Boron Nitride
National conference Organized by University Grants Commission on "Latest Developments in Basic and Applied Sciences" 10th January 2015, M. B. Patel Science College, Anand (Gujarat)

7) Shock Equation of States of Au: A Mean-Field Potential Approach
National conference on Condensed Matter Physics 27-28th March 2015 MIT University, Maniapal (Karnataka).

Contribution towards Society….

01 – M.Phil. (Entitled "Bulk and Surface Properties of Rubidium and Tin" by Dhaval D. Satikunvar)
01 – Ph.D. (Entitled "Thermophysical Properties of Noble Metals at Higher Pressure and Temperatures" by Rajani H. Joshi)

Whether objectives were achieved…. YES

Yes, it was fully achieved and briefly discussed in work done.

Achievements from the Project….

- As per original proposal, uniform and consistent to address high Temperature and high pressure vibrational properties of non-simple metals, like Cu, Ag and Au is proposed.
- Solid-Liquid phase boundary under pressure is investigated.
- Atomic transport properties in the liquid phase have been computed employing our newly proposed pseudopotential.

The Properties Studied in the Present Work are as Follows:

(i) Properties at high temperature:

- Cohesive energy as a function of volume.
- Phonon dispersion curve and phonon–density-of-state.
- Quasiharmonic Helmholtz free energy as a function of volume and temperature.
- Anharmonic total Helmholtz free energy as a function of volume and temperature.
- Linear thermal expansion coefficient.
- Isothermal bulk modulus.

- Adiabatic bulk modulus.
- Entropy.
- Enthalpy.
- Variation of specific heat at constant volume (C_V) with temperature.
- Variation of specific heat at constant pressure (C_P) with temperature.
- Temperature variation of thermodynamic Grüneisen parameter (γ_{th}).

(ii) Properties at high pressure:

- Pressure variation of thermodynamic Grüneisen parameter (γ_{th}).
- Static equation of state.
- Shock-Hugoniot (Dynamic) equation of state.
- Temperature along principal Hugoniot.
- Melting curve.
- Physical properties along Shock Hugoniot; viz. specific heat, enthalpy and Grüneisen parameter.

(iii) Liquid phase atomic transport properties:

- Inter-atomic pair-potential at different temperatures.
- Pair correlation function as a function of temperature.
- Variation of the dynamical structure factor at different wave vectors and as a function of temperature.
- The longitudinal current-current correlation function.
- Normalized velocity auto-correlation function.
- The self-diffusion coefficient as a function of temperature.
- Viscosity as a function of temperature.
- Cosine frequency power spectrum at different temperatures.
- Mean square displacement at different temperatures