Indian Institute of Technology Kanpur

Proposal for a new course

1. **Course No.:** MSExxx

2. **Course Title:** Computational Materials Thermodynamics

3. **Credits:** 3-0-0-0[9 credits]
Duration of course: Full semester (40 lectures)

4. **Proposing Department:** Materials Science and Engineering Department
Other departments which may be interested in the proposed course: ME, CHE, MSP, SEE

5. **Proposing Instructor:** Soumya Sridar
Other faculty members interested in teaching the proposed course: Dr. Krishanu Biswas, Dr. Kallol Mondal, Dr. Kaustubh Kulkarni, Dr. Rahul Sarkar, and Dr. Shivam Tripathi.

6. **Course Details:**

Objectives: The main objective of this course is to provide a foundation for using computational thermodynamics as a tool for alloy design and process optimization. Computational thermodynamics has become a reliable tool for accelerated materials discovery. A deeper understanding of this approach will be beneficial to efficiently solve metallurgical problems with computational techniques rather than brute-force experiments involving high material costs and energy consumption. This course is intended to provide an overview of topology and methods for phase diagram construction, understand the fundamental principles of phase and property diagram calculations with thermodynamic database structure, and modern data-driven techniques for accelerating phase diagram development. The course will also include hands-on experience in using the appropriate software tools to perform thermodynamic calculations relevant to design and optimization, including thermodynamic database development. It is expected that after going through this course, a student will be able to comprehend scientific literature and will be equipped to perform research using this approach.

Contents:

S. No.	Topic	Lectures
1	**Review of basic thermodynamics and phase diagrams**	
	Thermodynamic definitions and equilibrium conditions	2
	Topology of ternary and multicomponent phase diagrams	1
	Methods of phase diagram construction	2
2	**Overview of computational thermodynamics**	
	Introduction to computational thermodynamics	1
	Linkage between computational thermodynamics and other modeling techniques	1

3	**Gibbs energy models for different phases**	
	Models for pure elements, stoichiometric phases and gases	1
	Models for random substitutional solutions and their extrapolation	3
	Sublattice formalism and its applications	5
	Models for magnetic ordering and ionic liquids	1
4	**Computational thermodynamics tools and databases**	
	Introduction to computational thermodynamics tools	1
	Structure and assembly of thermodynamic databases	3
5	**Hands-on computational thermodynamics calculations**	
	Calculation of binary phase diagrams and property diagrams	1
	Calculation of different sections (isothermal, isopleth, liquidus projection) for ternary systems	2
6	**Gibbs energy model parameter optimization**	
	Types of experimental data and its critical evaluation	1
	Ab initio assisted thermodynamic input data generation	3
	Gibbs energy model parameter optimization steps and practices	4
	Model parameter optimization for Ni-Cr system: A case study	2
7	**Modern alternate approaches for computational thermodynamics**	
	Atomistic simulations for implementing computational thermodynamics	2
	First-principles-only phase diagram of Ni-Al system: A case study	1
	Machine learning for computational thermodynamics and related tools	3
	Total	**40**

7. **Prerequisites:** Basic Materials course on thermodynamics

8. **Short summary of the course content:**

Computational thermodynamics combines classical thermodynamics with mathematical modeling for accelerated and efficient material discovery and process optimization. This course will begin with reviewing the basic thermodynamic terms along with understanding the topology, and construction of phase diagrams. This will be followed by introducing computational thermodynamics and the Gibbs energy models for various phases, such as pure elements, gases, liquids, and solid solutions, which will be discussed in detail as they are crucial for phase diagram determination. Different software tools for implementing computational thermodynamics will be introduced along with the structure of Gibbs energy databases, which will be followed by hands-on experience in performing calculations using the relevant software. This will be followed by a comprehensive introduction to Gibbs energy model parameter optimization, the main crux for developing databases for thermodynamic calculations with a case study including thermodynamic data generation using first-principles calculations. Further, the modern techniques for implementing computational thermodynamics for rapid phase diagram determination, such as ab initio methods and machine learning approaches, will be elaborated with suitable examples and tools.

9. **Textbooks and Reference Book:**

1. CALPHAD (Calculation of Phase Diagrams): A Comprehensive Guide, N. Saunders and A.P. Miodownik, Pergamon Press, 1998 (Textbook)
2. Computational Thermodynamics: The Calphad Method, H.L. Lukas, S.G. Fries, B. Sundman, Cambridge University Press, 2007 (Textbook)
3. Phase Equilibria, Phase Diagrams, and Phase Transformations: Their Thermodynamic Basis, M. Hillert, Cambridge University Press, 2007 (Reference book)
4. Computational Thermodynamics of Materials, Z. K. Liu, Y. Wang, Cambridge University Press, 2019 (Reference book)

Date: 03/02/2025 **Proposer:** Soumya Sridar

Date: _____ **DUGC/DPGC Convener:**

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The course is approved/not approved.

Chairman, SUGC/SPGC

Date: _____