THERMODYNAMICS CONSORTIUM

A triumvirate of experimental thermodynamics, structural investigation and theory/computation

THE NEED

Thermodynamics forms the fundamental underpinning of reactivity, transformation, and stability. It controls synthesis, corrosion and degradation, environmental transport, catalysis, and biological reactivity.

In the materials field, the new compounds, polymorphs, hybrid organic-inorganic hybrid materials and metal organic frameworks, high-entropy alloys, multiphase and nano materials, attained by a variety of nonequilibrium synthesis and processing methodologies, has outrun available thermodynamic data. In the geological and environmental sciences, similar needs for thermodynamic data for complex minerals exist. The excitement of new chemistry in planetary systems, both in our solar system and beyond, requires a broad scale thermodynamic approach. The needs of materials science, earth and planetary science, and environmental science are both overlapping and complementary.

The rapid developments in industry have resulted in an increasing need for improved and new materials, better ways to characterize them and to study their properties, in order to explain different phenomena and process failure on a large scale. Thus fundamental and applied thermodynamics are being brought even closer together, making narrowly defined “pure science” a thing of the past and interdisciplinary studies, novel and hybrid materials, and broad collaborations across academia and industrial R&D the new future.

The capabilities and interest for thermodynamic measurements have been on the rise again after years of decline resulting in new commercially avaliable thermal analysis equipment and the ability to make accurate cryogenic heat capacity measurements.

The developments in experimental thermochemistry are paralleled by rapid progress in computational methods. These integrate state-of-the-art calculations based on density functional theory (DFT), new simulation methods for characterizing energy and free energy landscapes.

The experimental techniques for elucidating details of structures of solids at the molecular, nano, and meso scale have improved immensely, led by, but by no means limited to, experiments involving diffraction, scattering, and spectroscopy at synchrotron and neutron sources.

THE GOALS

- To elevate awareness of how useful and essential modern thermodynamics is to many fields and to provide easy access to collaborations.
- To exchange best practices and scientific discoveries among the participants.
- To guide and support young researchers using the members’ vast experience in experimental and computational thermodynamics, and in structural studies.
- To work with other database developers and users to create an interactive, growing and easily updated reference database of thermodynamic parameters for complex materials.

https://www.thermocon.org

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THE GOALS (continuation)

➢To enhance communications with manufacturers of scientific measurement equipment and industry in general, who will respond to the needs of their customers.

➢ To stimulate the development of large multi-investigator proposals and explore joint opportunities for funding.

➢ To bring together computational thermodynamicists, representing both first principles molecular level calculations (DFT, MD etc.) and phase diagram computation (CalPhaD, big data, materials genome, etc.), crystallographers, spectroscopists and other people working on complex structures and reactivity to coalesce a truly interactive consortium.

➢ To organize workshops, short courses, targeted sessions at technical conferences, and topical special issues of journals (e.g. ACS, MS&T, MRS, Goldschmidt, AGU, GSA)

WHO WE ARE

Experimental thermodynamicists who interact with a wider circle of computational and structural scientists to understand the fundamental thermodynamics of complex materials and apply this understanding to a rich variety of scientific and technological problems.

➢ over 180 participants
➢ 15 countries
➢ more than 50 universities, institutes and national labs
➢ 5 companies
➢chemists, physicists, materials scientists, chemical engineers, and earth and planetary scientists

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