



TECHNION – Israel Institute of Technology
Faculty of Mechanical Engineering

הרצאת אורח ע"ש ישראל פולק - תש"ע
Israel Pollak Distinguished Lecture series 2009

הנדן מוזמן/ת להרצאה סמינריונית של הפקולטה להנדסת מכונות, שתתקיים ביום ב' 19.10.09 (א' בחשון, תש"ע), בשעה 14:30, בחדר 641 בבניין ליידי-דייויס.

ירצה:

Dr. Michael Frenkel
Thermodynamics Research Center
Thermophysical Properties Division
National Institute of Standards and Technology
Boulder, Colorado, USA

על הנושא:

Thermodynamic Approach: Powerhouse for Science and Engineering

להלן תקציר ההרצאה:

The power of phenomenological and statistical thermodynamics and the unique role of thermochemical and thermophysical data will be illustrated by a variety of studies in very diverse scientific and industrial fields ranging from conformational analysis to optimization of high-tech space and mass-scale chemical technologies and from data communications to data expert systems for chemical process design.

The results of an application of bomb calorimetry combined with chemical equilibria and NMR studies to diastereomers and conformers of acyclic, monocyclic, and bicyclic alcohols will be discussed to analyze predictive capabilities of group contribution methods for organic compounds with various degrees of 'rigidity' of their carbon skeleton.

The simultaneous application of adiabatic calorimetry and IR spectroscopy methods for studying 'cage' hydrocarbons will be described in the context of direct determination of the nature of the plastic crystalline state.

New computational techniques for calculation of the heat capacity of mixing in the ideal gas state for organic compounds existing as mixtures of conformers and tautomers will be illustrated for cyclohexanol and cyclohexanone molecules. The obtained results were used for mathematical modeling of the process of dehydrogenation of cyclohexanol, a major stage in mass-scale production of caprolactam (monomer for Nylon production).

An application of the Gibbs minimization method for multicomponent multiphase analysis of complex equilibria will be illustrated for 'rocket fuel-coolant' systems to determine the most efficient coolants and optimal multistage technology to decrease the temperature of the products of fuel combustion.

Efforts in standardization of thermodynamic data communications will be reviewed. The basic principles, scope, and description of major structural elements of ThermoML- an XML-based emerging IUPAC standard for storage and exchange of experimental, predicted, and critically evaluated thermophysical and thermochemical property data will be discussed.

The first full-scale software implementation of the dynamic data evaluation concept {*ThermoData Engine* (TDE)} will be described for thermophysical and thermochemical property data.

בברכה,

ד"ר רנה ואן האוט
מרכז הסמינרים

המארח: פרופ' גרשון גרוסמן



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הנד מוזמנת/ת להרצאה סמינריונית של הפקולטה להנדסת מכונות, שתתקיים ביום ד' 21.10.09 (ג' בחשון, תש"ע), בשעה 14:30, בחדר 641 בניין ליידי-דייויס.

ירצה:

Dr. Michael Frenkel
Thermodynamics Research Center
Thermophysical Properties Division
National Institute of Standards and Technology
Boulder, Colorado, USA

על הנושא:

Global Information Systems in Science:
Application to the Field of Thermodynamics

להלן תקציר ההרצאה:

Global Information Systems can be defined as information systems designed to collect, process, integrate, evaluate, and communicate the entire "body of knowledge" pertaining to a field and to support any application requiring this knowledge in an "on-demand" mode with definitive information quality assessments.

Recent advances in computer hardware technology, development of relational data management systems capable of reliably supporting storage of enormous amounts of information pertaining to specific areas of science, new interoperable means of standardizing data communications based on the Extensible Markup Language (XML) ontologies, new generation software expert systems, and secure on-line networks have created unprecedented opportunities for defining and implementing a new paradigm of Global Information Systems in Science. Global Information Systems have a profound impact on the scientific discovery process, industrial development, and knowledge communication.

Within the last 10 years, one of the first Global Information Systems in Science has been developed for the field of Thermodynamics (Thermo Globe) at the Thermodynamics Research Center (TRC) of the U. S. National Institute of Standards and Technology (NIST). The components of this system include software tools for mass-scale data capture (Guided Data Capture Software), a comprehensive data storage facility (SOURCE Data Archival System), the NIST/TRC Data Entry Facility, a data communication standard (Thermo ML – IUPAC standard for thermodynamic data communications), data "reader" software (Thermo ML opener into Microsoft Excel), expert system software (NIST Thermo Data Engine), and a Web communication portal (NIST Web-Oracle data dissemination channel).

The role and principal structure of all the components will be discussed with the emphasis on the profound impact of the Thermo Globe implementation on various areas of research and engineering including, but not limited to, efficiency of information delivery, journal publication quality, and chemical process design

בברכה,

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מרכז הסמינרים

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