Editorial



In August 2006, more than 350 scientists from all over the world will convene in Vienna, Austria, to discuss various issues and topics in thermoelectricity at the International Conference on Thermoelectrics, ICT06. Recent years have seen a strong worldwide scientific and technological commitment toward a new generation of thermoelectric devices. We all know that *thermoelectrics* has been defined as the science and technology associated with thermoelectric power generation and refrigeration. A thermoelectric converter is formed by connecting two semiconducting materials (thermoelements) at a junction to form a thermocouple. When the junction is maintained at a temperature that differs from the ambient, a voltage is established across the open ends of the thermocouple (Seebeck effect), and if the circuit is closed with a resistance load an electric current flows in the circuit. The device operates as a generator converting the flow of heat into electrical power. Conversely, when a current is supplied to the thermo-

couple, heat is pumped from one junction to the other, depending on the direction of current flow (Peltier effect), and the device operates as a refrigerator. In practice, a large number of thermocouples are connected electrically in series and thermally in parallel to form a module. The module is the active component of a thermoelectric generator or refrigerator.

The large amount of abstracts received for ICT06 emphasizes the considerable academic and industrial interest in the conference theme. Thermoelectric materials cover a large spectrum of applications relevant to civil markets, space, electronic, or military markets. Major advantages over conservative competitive systems are, in particular: high reliability, silent motionless operation, saving waste energies, and being environment friendly. Science and technology of thermoelectric materials (multicomponent and multiphase materials) require a multidisciplinary approach comprising expertise in materials chemistry, physics, metallurgy, and ceramics, in experiment and theory, in electrical and device engineering, and so forth. Accordingly, the interaction among research/technology/industrial applications needs to be strongly developed, if large-scale industrial and technological development is expected. Major objectives of research activities are currently focused on topics that may lead to significant improvements of the efficiency of vehicle-propulsion systems. Hence, more advanced hybrid power trains with internal combustion engines or fuel-cell systems are under investigation. This also includes storage of electric energy on board with next-generation supercapacitors and/or lithium-ion batteries. Furthermore, electric power generation on board by means of fuel-cell-driven auxiliary power units is of major interest. Although such technologies will lead to improved propulsion efficiencies, waste heat is still generated even in case of the best fuel-cell power train. Due to the steady increase in electrification of vehicles, the demand for electric power is increasing on the one hand, and the electrical on-board infrastructure is extending, obviously opening the door for the integration of electrical devices for waste heat recovery.

From the conference contributions it is interesting to see that design of thermoelectric materials shows an increasing demand for reliable phase diagrams, phase stabilities, and diffusion parameters. Thermochemical calculations using the CALPHAD approach in conjunction with key experiments have shown their strengths to provide these data in reasonable time even for multicomponent materials. As a complementary tool, ab initio techniques, that is, density functional theory (DFT) calculations, nowadays are capable of providing not only enthalpy data with high accuracy and with moderate computational efforts, but also phonon dispersion, elastic constants, electronic structure, Fermi surfaces, magnetic ground states, and so forth, defining relative phase stabilities and physicochemical properties. The new computational tools are an indication of the importance of modeling and simulations.

It is my belief that such a combined and balanced approach comprising experimental and computational techniques will ensure a sound physicochemical basis for successful development and design of advanced engineered (thermoelectric) materials.

Further details on ICT06 can be gathered from the website http://www.univie.ac.at/ICT06.

Peter Rogl Associate Editor *Journal of Phase Equilibria and Diffusion*