

Abstract Submitted to the  
IICAM Workshop on Correlated Thermoelectricity  
25 - 30 September, 2005  
Hvar, Croatia

## **Clathrates - from hydrate clathrates to intermetallics with thermoelectric properties**

Peter Rogl

*Institut für Physikalische Chemie, Universität Wien, A-1090 Wien, Austria*

True clathrates are considered to be compounds that have no pair-wise bonds between framework and neutral guest atoms or species. Most clathrate compounds for thermoelectric use, however, are intermetallic materials built from face-sharing cages of Si, Ge or Sn atoms which are tetrahedrally  $sp^3$  bonded, the cages enclosing the guest species. Experimental evidence supports rather the interaction between the inclusion atom and the entire cage, the guest atoms behaving as charge donors. In many cases filler atoms do not reside at the centre of the large cages but are arranged in split atom positions with smeared out electron densities. Based on this behaviour a charge-balanced Zintl phase model was earlier suggested for these compounds, which despite its simplicity proved remarkably well applicable to the large group of complex clathrates in general. The present paper focuses on a systematic study of clathrate formation, clathrate structures and bonding in clathrate materials. The analysis shows the difficulties in preparation and design of clathrate compounds at a given electron/atom concentration. Validity and shortcomings of the Zintl concept for clathrates will be outlined. Nevertheless the correlations obtained, although not complete for many systems, may provide useful in defining compositional regions of interest for further search for novel clathrate materials with interesting thermoelectric properties.

*Keywords :* Clathrates, Crystal Chemistry, Thermoelectric Properties