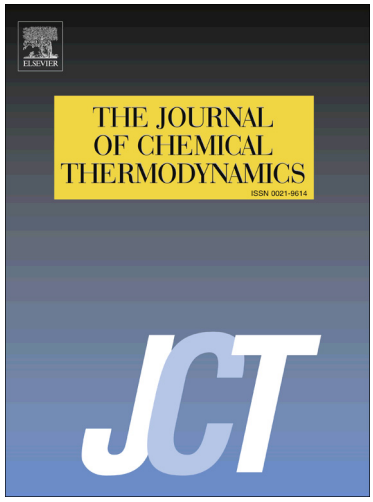

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Chemical bonding and thermodynamic properties of gallium and indium monochalcogenides

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Abstract

Monochalcogenides of heavier Group 13 (AIII) elements represent a unique family of compounds which, unlike the corresponding sesquichalcogenides, do not follow the classical valence concept. Their low-dimensional structures and semiconducting transport characteristics make them prospective candidates for various applications such as nanoelectronics, photonics and thermoelectric conversion. On the other hand, the variety of the respective phase diagrams involving several coexisting phases in narrow compositional ranges and high volatility of the components represent a challenge for their reproducible synthesis. In this study we explore the thermodynamic properties of In and Ga monochalcogenides by ab-initio density functional theory calculations of enthalpies of formation, low temperature heat capacity measurement to assess the standard entropies and differentials scanning calorimetry to obtain the temperature dependence of heat capacity above the reference temperature.