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## Repository for phase-based data

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### ABSTRACT

Computational tools allow efficient evaluation of materials properties and behavior and are at the core of Integrated Computational Materials Engineering. All these tools rely on experimental data or results from calculations at lower length scales for the development of model parameters and/or verification of the results. Classical data collection from publications by retyping or digitizing is time consuming and leads to errors in the captured data. Depending on the task, data users may prefer evaluated data, which are usually communicated in publications, whereas others prefer raw data which are rarely communicated in publications. Appropriately designed data and file repositories can provide users with data that are best suited for their needs. In the fast developing world of information technology, these repositories must be flexible enough to accommodate evolving data needs while being selfconsistent in providing unique identifiers for materials and offer valuable information for a variety of applications. NIST is developing prototype repositories and data schemas with focus on data that are needed by the CALPHAD community. The materials property specifications and materials ontologies explored in this study and the current state of the repositories will be presented.