

The Material Genome Initiative, NIST and the Materials Innovation Infrastructure for Data, Repositories, and Standards

Ursula Kattner¹, Carelyn Campbell¹, Benjamin Burton¹, Eric Lass¹ and Laura Bartolo²

¹ National Institute of Standards & Technology

² Kent State University

NIST is playing a lead role in developing the critical models, tools, standards, and data required to meet the needs of the national Materials Genome Initiative (MGI). Focusing on essential methods for the development and integration of MGI's Materials Innovation Infrastructure (MII), NIST is building three data repositories modeled after the NIST Interatomic Potentials Repository <<http://www.ctcms.nist.gov/potentials/>>. The first repository contains a collection of files used in first principles calculations. The second repository includes data files used with the CALPHAD method such as TDB functional description files and POP files and EXP files with experimental and calculated data for the optimization of the functional descriptions and plotting of the results, respectively. The First Principles and CALPHAD repositories, organized by systems, both contain original work with files that are software specific. The third repository is a general data repository that includes additional background information from original articles needed to critically evaluate the experimental and calculated data in the First Principles and CALPHAD repositories. As part of MII, the NIST repositories, designed to accommodate evolving data needs as well as to provide unique identifiers for phases and materials, will offer valuable information for a range of applications.

Keywords: materials data, materials engineering research, materials databases, materials education