

Abstract Submitted
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The Structural Database¹ NIKOLAI ZARKEVICH, D.D. JOHNSON,
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Champaign. — A Structural Database can be used as a universal tool for global
accumulation and integration of structural and energy data from different methods,
people, and places. It allows data mining and data validation by direct comparison
of structural data from different sources. Being combined with multi-scale methods
(e.g., ThermoToolkit), it can significantly reduce the cost of materials design. We
exemplify these and other benefits of the Structural Database, and demonstrate
its working prototype, available at <http://data.mse.uiuc.edu>. This database is a
product of multi-disciplinary research involving Physics, Computer Science, and
Materials Science and Engineering.

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