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The role of Wang-Landau sampling in materials development[1]

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An understanding of the thermodynamic behavior of materials as well as the prediction of the properties of "materials by design" often depends upon knowledge of the free energy of the system under study. Computer simulations offer a powerful tool for such investigations, but traditional methods often suffer from long time scales and metastable states due to the roughness of the free energy landscape. Wang-Landau sampling[2] is a powerful alternative to traditional Monte Carlo algorithms which can alleviate many such problems. We will review the Wang-Landau algorithm and discuss various implementations as well as possible application to materials development.

[1]Supported by the National Science Foundation.

[2]F. Wang and D. P. Landau, Phys. Rev. Lett. 86, 2050 (2001); F. Wang and D. P. Landau, Phys. Rev. E 64, 05610 (2001).