Abstract Submitted for the MAR14 Meeting of The American Physical Society

**Basis Function Sampling for Material Property Computations** JONATHAN K. WHITMER, CHI-CHENG CHIU, Materials Science Division, Argonne National Laboratory, ABHIJEET A. JOSHI, Department of Chemical Engineering, University of Wisconsin–Madison, JUAN J. DE PABLO, Institute for Molecular Engineering, University of Chicago — Wang–Landau sampling, and the associated class of flat histogram simulation methods, have been particularly successful for free energy calculations in a wide array of physical systems. Practically, the convergence of these calculations to a target free energy surface is hampered by reliance on parameters which are unknown *a priori*. We derive and implement a method based on orthogonal (basis) functions which is fast, parameter-free, and geometrically robust. An important feature of this method is its ability to achieve arbitrary levels of description for the free energy. It is thus ideally suited to *in silico* measurement of elastic moduli and other quantities related to free energy perturbations. We demonstrate the utility of such applications by applying our method to calculation of the Frank elastic constants of the Lebwohl–Lasher model.

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Date submitted: 15 Nov 2013

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