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**Electronic structure from Maximum Entropy optimization: Applications to band energy and electronic force computation**[1] HIRO SHIMOYAMA, PARTHAPRATIM BISWAS, The University of Southern Mississippi — We apply a new entropy optimization scheme to study the electronic density of states for complex disordered materials from a knowledge of spectral moments. We employ the Shannon entropy functional in our work and maximize it subject to the moment constraints to construct the spectral distribution of large Hamiltonian matrix[1]. We illustrate the efficiency and the usefulness of the method by reconstructing a number of exact functions, which are difficult to reproduce by other function reconstruction techniques. The local and global convergence properties of the resulting distribution is studied and the band energy and Fermi level are computed with a high degree of precision. An extension of this method to calculate electronic forces is presented for the purpose of using in large-scale molecular dynamics simulation of materials.

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