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Moment based approach to electronic structure calculations: applications to ordered and disordered systems[1] HIRO SHIMOYAMA, The University of Southern Mississippi, PARTHAPRATIM BISWAS, University of Southern Mississippi — We solve the classical moment problem via maximum entropy optimization to calculate the electronic density of states for ordered and disordered solids. The method employs the Shannon entropy functional and maximize it subject to the moment constraints to construct the spectral distribution of large Hamilton matrix. We illustrate the efficiency and usefulness of the method by applying three candidate systems: a crystalline semiconductor; an amorphous material; and a completely disordered system via tight-binding Anderson model Hamiltonian. The band energy and Fermi level are computed from the reconstructed density of states with a high degree of precision. A possible extension of this method to calculate electronic forces is also discussed.

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