

Abstract Submitted
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Sum rule constraints on model dielectric functions ERIC L. SHIRLEY, KEITH GILMORE, NIST — The f-sum rule, Kramers-Kronig relations, orthonormality of Kohn-Sham orbitals and properties of the one-particle density matrix all dictate sum rules that can be used to maximize the physicality of model dielectric functions. In this talk, we wish to discuss aspects of the zeroth-frequency moment of the Lindhard polarization function that appear relatively unexploited in earlier work. We shall assess the effects on low-frequency dielectric properties and electron lifetime damping effects. We shall discuss the origin of various sum rules, a proposed method to implement them, and numerical results that can be obtained in a range of materials.

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