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Density and Spectral-Density Matrices in Atomistic-Scale Models[1] STEVEN VALONE, Los Alamos National Laboratory — Density matrices for the states of atoms appear from the construction of a model referred to as the Fragment Hamiltonian (FH) model. The FH model is not dependent on construction of one-electron as a prelude to the atomistic level. Rather a density matrix of occupation numbers of the integer charge states is composed directly from a many-electron point of view to represent the state of each atom or fragment in a molecule or material. The properties of these density matrices comply with those general density matrices. Two particular properties are explored. One property that is unique to the FH model is that the coefficients of the occupancy density matrix can be transformed into functions of more familiar variables, such as net charge and ionicity that play a central role in regulating charge flow in a molecule or material. The second property is that the concept of a spectral density matrix can be defined as an extension of the occupancy density matrix and again is utilized in a manner that is analogous to the role of that concept in one-electron theories of electronic structure. The construction and functionalities of both density matrix concepts are illustrated through examples from idealized systems such as one-dimensional chains.

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Steven Valone
Los Alamos National Laboratory

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