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**Electrical conductivity of warm expanded aluminum** GERALD FAUSSURIER, CHRISTOPHE BLANCARD, PATRICK RENAUDIN, CEA, PIER-LUIGI SILVESTRELLI, Università di Padova, CEA COLLABORATION, UNIVERSITÀ DI PADOVA COLLABORATION — The electronic and ionic structures of warm expanded aluminum are determined self-consistently using an average-atom formalism based on density-functional theory and Gibbs-Bogolyubov inequality. Ion configurations are generated using a least-square fit of the pair distribution function deduced from the average-atom model calculations. The electrical conductivity is computed from the Kubo-Greenwood formula for the optical conductivity implemented in a molecular dynamics scheme based on density-functional theory. This method goes beyond the Ziman approach used in the average-atom formalism. Moreover, it is faster than performing quantum molecular dynamics simulations to obtain ion configurations for the conductivity calculation. Numerical results and comparisons with experiments are presented and discussed.

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