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Nuclear Thermal Motion Driven Adiabatic Electron States Thermalization and the Induced Phase Transition From Insulator To Metal in Warm Dense Matters DONGDONG KANG, YONG HOU, CHENG GAO, JIAOLONG ZENG, JIANMIN YUAN, National University of Defense Technology
— In warm dense matter(WDM), the thermal motion energy of a nucleus may be comparable to its coupling energy with the neighbor nuclei and comparable to the valence electronic orbital motion energy. As the much small mass of electrons, the fluctuations of the electron orbitals are almost adiabatic dynamical changes with nuclear motion. The electronic and nuclear structure of warm and dense He and Ar are simulated by using the density functional based molecular dynamics method. The nuclear thermal motion driven adiabatic thermalization of the electron states, depression of the energy band gap and even phase transitions of electron states from insulator to metal are predicted when the nuclear thermal motion energy is comparable to the coupling energy between the neighboring atoms as well as to the valence electronic orbital motion energy. These kind of nuclear thermal motion driven adiabatic electronic states from insulator to metal phase transition occurs at much lower temperatures than the normal thermal collision excitation in low density and high temperature gases.

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