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Ab initio evidence for nonthermal characteristics in ultrafast laser melting CHAO LIAN, Chinese Academy of Sciences (CAS), SHENGBAI ZHANG, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, SHENG MENG, Chinese Academy of Sciences (CAS) — Laser melting of semiconductors has been observed for almost forty years; surprisingly, it is not well understood where most theoretical simulations show a laser-induced thermal process. Ab initio nonadiabatic simulations based on real-time time-dependent density functional theory reveals for the first time intrinsic nonthermal melting of silicon, at a temperature far below thermal melting temperature of 1680 K. Both excitation threshold and time evolution of diffraction intensity agree well with experiment. Nonthermal melting is attributed to excitation-induced drastic changes in bonding electron density, and subsequent decrease in melting barrier, rather than lattice heating as previously assumed in the two-temperature models.

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