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Extended First-principles molecular dynamics toward high temperature WEI KANG, SHEN ZHANG, PING ZHANG, X.T. HE, Center for Applied Physics and Technology, Peking University — An extended first-principles molecular dynamics method (ext-FPMD)[1], which incorporates an analytical formula of the contribution of high energy electrons into the Kohn-Sham-Mermin scheme, is proposed to significantly improve the efficiency of finite-temperature density functional theory for hot dense plasmas while still maintaining the numerical accuracy. The new method eliminates the explosively growing computational costs at high temperature up to thousands of electron volts, and naturally returns to the original Kohn-Sham-Mermin scheme when the temperature is close to zero. It thus consistently deals with materials from 0K to about 2000eV, which is important to the application of inertial confinement fusion. Compared with other first-principles methods for dense plasmas, the newly devised method also keeps the information of electronic structures at high temperature, which gives it an edge in the future study of transport properties.

[1]S. Zhang, W. Kang, P. Zhang, and X. T. He, Physics of Plasmas **23**, 042707 (2016)

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