DFT-WPMD method for nonideal plasma and warm dense matter simulations.

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A combination of Density Functional [1] and Wave Packet Molecular Dynamics (WPMD) [2-5] methods is proposed to simulate the thermodynamics and the electronic dynamical properties of non-ideal plasmas and warm dense matter. In this approach we use the non-antisymmetrized single Gaussian wave packets to represent electrons and point-like particles for ions. The kinetic and electrostatic energy contributions for electrons are calculated within the WPMD model, whereas the exchange-correlation energy and its derivatives with respect to the dynamic variables is evaluated on a space mesh. Constraining boundary conditions with a harmonic wall potential are used for wave packets to prevent wavepacket spreading [6].

Although more computationally demanding than the original WPMD method, the proposed technique allows one to account for both exchange and correlation effects within the non-adiabatic approach. The use of GPU acceleration for computing the exchange-correlation energy contribution turns to be quite effective and compensates the extra computational costs.

In this work we benchmark the DFT-WPMD with the basic local spin density approximation with (LSDA) exchange-correlation functional against test systems (homogenous electron gas, atomic and molecular hydrogen) and the nonideal hydrogen plasma in the temperature range of $T = 2 \times 10^4$–5×10^5 K and the nonideality parameter values $\Gamma = 0.01$–6. The results are compared with the classical molecular dynamics, the original wave packet molecular dynamics (WPMD) including the version with antisymmetrized wave packets [2] and the Path Integral Monte Carlo (PIMC) [7] methods.

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