O.40 Extended-DFT model for high temperatures simulations in ABINIT and applications to warm dense aluminum and boron

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The extended first-principle molecular dynamics (FPMD) model introduced by Zhang et al. [4] has been implemented within ABINIT [2] and is ready to merge. This model allow to perform quantum molecular dynamics (QMD) simulations at high temperature, bypassing the well-known orbital wall [1]. QMD simulations can be done smoothly in the full range of temperatures from cold condensed matter to hot plasmas (>10 keV), passing by the warm dense matter regime. At high temperature, a minimum of Kohn-Sham is kept, allowing for deep ionization effects to manifest, such as the Shottky anomaly, at contrast with orbital-free approches, where this effect is absent.

After a reformulation of the model in terms of Gaussian packets and with analytical evaluations of the high energy electron contributions, we present applications to aluminum and boron. Simulations for multiple isochores from few Kelvins to thousands of eVs, result in Hugoniot transformation very close to the FPEOS model [3] for a much lower computational intensity. The Kubo-Greenwood formulation for optical properties in this context is addressed.

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