

# A new two thermostat formulation of ab-initio molecular dynamics

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The problem of heating the wave functions in a Car-Parrinello simulation is solved in a more rigorous way, based on a consistent description of effective mass tensor and the thermostat feedback. The new thermostat is active only when the electrons heat above the Born Oppenheimer kinetic energy. Its implicit perturbation on the dynamics is minimized by counteracting forces. The formulation puts the Car-Parrinello method on a more rigorous footing, in that the accuracy is not dominated by the size of the fictitious electron mass, but by the accurate representation of the effective mass tensor.