

Illustrations of Some Implemented Examples with Adaptive-Timing, Electronic-Stopping and Electron-Phonon Coupling Model in TurboGAP

Uttiyarnab Saha

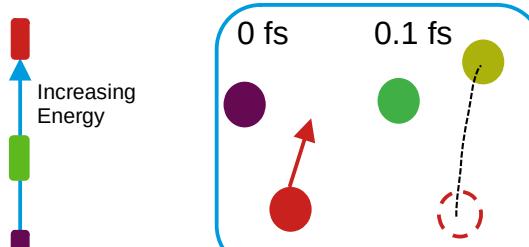
Department of Applied Physics
Aalto University, Finland

To select a time step (unit of time is fs):

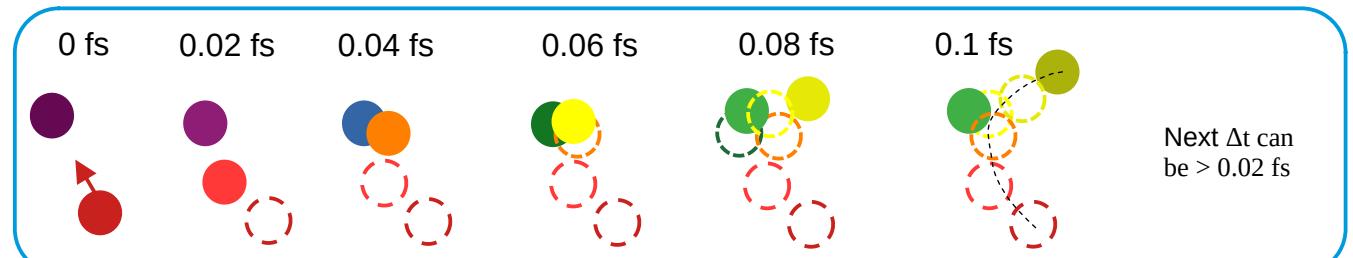
The basic relation $\Delta x = v\Delta t$ is suitable in normal situations. In radiation cascades the atoms experience very strong collisions where this time step could be very long.

Then, we will actually need $\Delta x \leq 0.0001 \text{ \AA}$ to see the exact trajectories and energy sharing by the atoms during cascade progress.

We use a x_{\max} criterion to allow maximum possible distance an atom can move in a time step and also a e_{\max} criterion to allow maximum possible change in K.E of an atom.



Fixed time step



Adaptive time step – with smaller Δt at high E and larger time steps at low E

The displacement of atoms in cascades take place through binary elastic collisions. The nuclear energy loss is important in damage calculations.

But there is electronic energy loss too, at all energies.

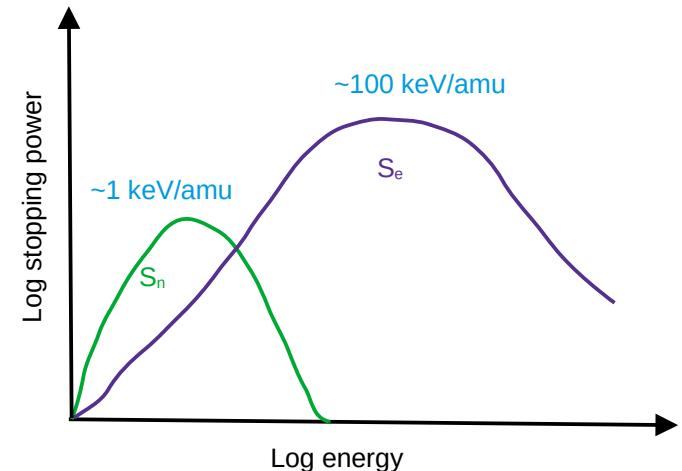
Only damage energy part of K.E of PKA is responsible for damage creation.

The damage energy depends on K.E of PKA and also on the types of the elements (PKA and the target) through the characteristic electronic energy loss.

In the past, we used to do MD with $T_{\text{dam}} = E_{\text{PKA}} - E(\text{el})$ as the PKA energy, calculated analytically from energy partition theory or from the data from SRIM software.

But advances allow for real-time EEL calculations while simulating a cascade in MD. There are a few approaches possible.

- S_e (in units eV/ \AA) is obtained as a function of E_{ion} from SRIM-2013.
- User provides a lower cut off energy (few tens of eV, usually) and the name of stopping data file.



Modify the forces as

$$\vec{F} = \vec{F}^0 - S_e \frac{\vec{v}}{v}$$

Adaptive time

For the user ::

Simple input keywords starting with the word 'adapt':

```
adaptive_time = .true.  
adapt_tstep_interval = 1  
adapt_tmin = 1.0e-07  
adapt_tmax = 0.1  
adapt_xmax = 1.0e-4  
adapt_emax = 50.0
```

Electronic stopping

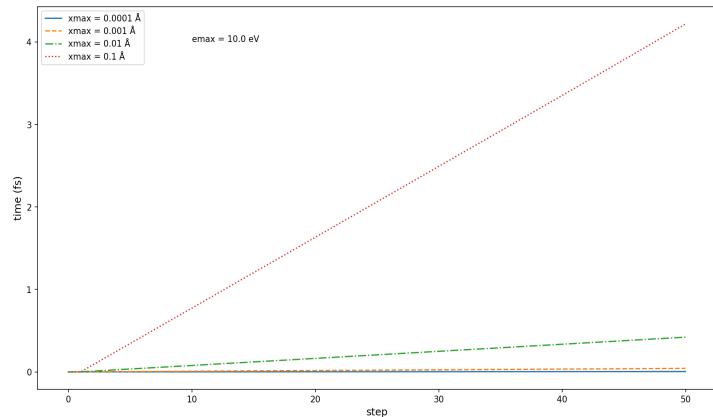
For the user ::

Simple input keywords

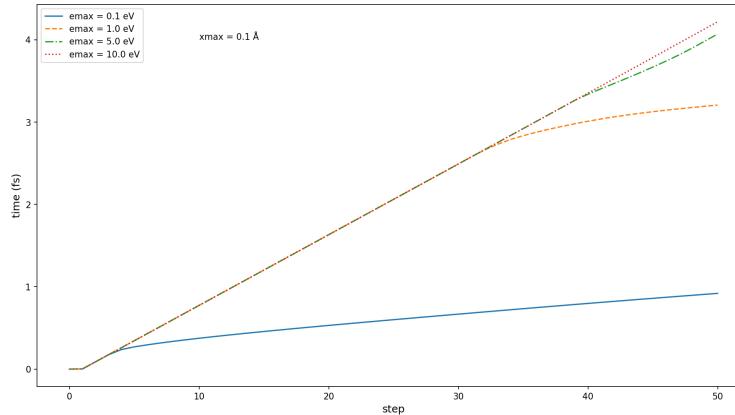
```
electronic_stopping = .true.  
eel_cut = 5.0  
eel_freq_out = 10  
estop_filename = 'stopping-data-file.txt'
```

Sensitivity of adaptive timing to maximum distance and energy criteria

Sensitivity to xmax



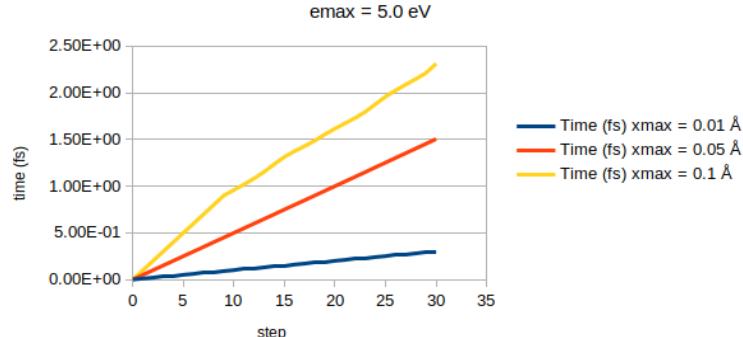
Sensitivity to emax



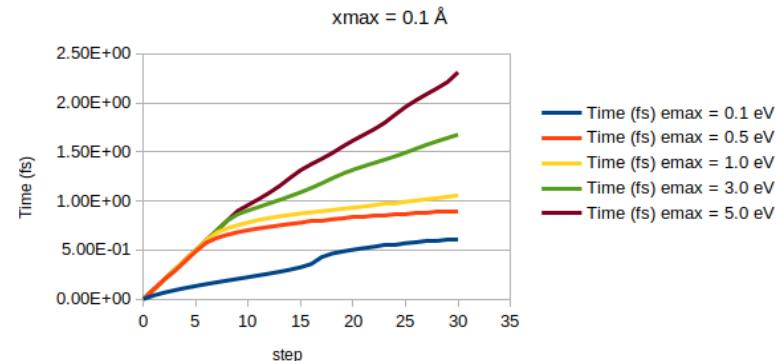
Sensitivity of time steps to xmax and emax in a binary collision simulation

Two Si atoms at $r_1 = (10.0, 10.0, 10.0)$ and $r_2 = (13.0, 10.0, 10.0)$ with $v_{1x} = 1.0 \text{ \AA/fs}$, $v_{1y} = 0.0$, $v_{1z} = 0.0$ and $v_{2x} = -1.0 \text{ \AA/fs}$, $v_{2y} = 0.0$, $v_{2z} = 0.0$ using Si (not stiffened) GAP potential.

Binary Collision using TurboGAP



Binary Collision using TurboGAP



Some Simulations with Fixed and Adaptive time steps

Silicon with 4096 atoms – one atom is given ~100 eV energy

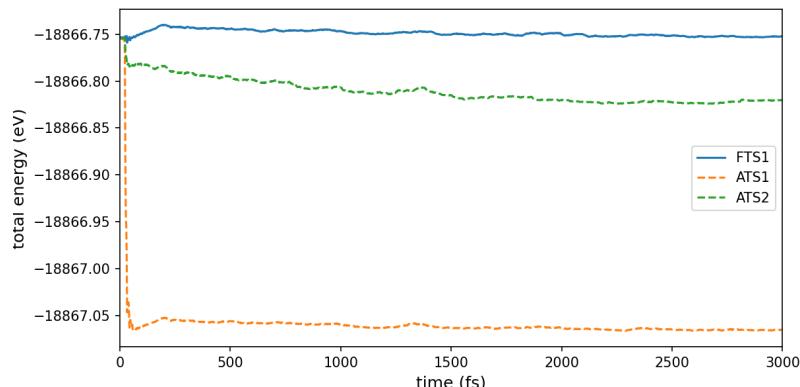
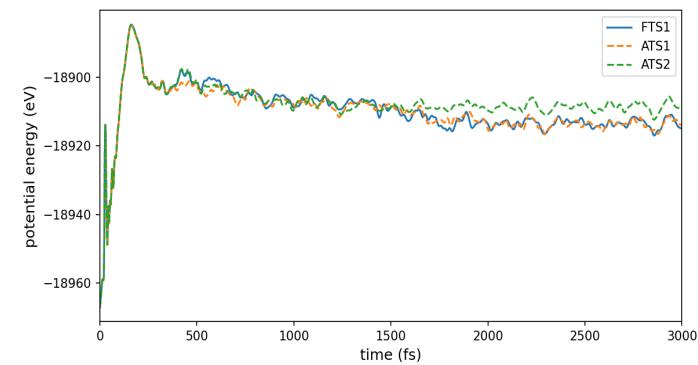
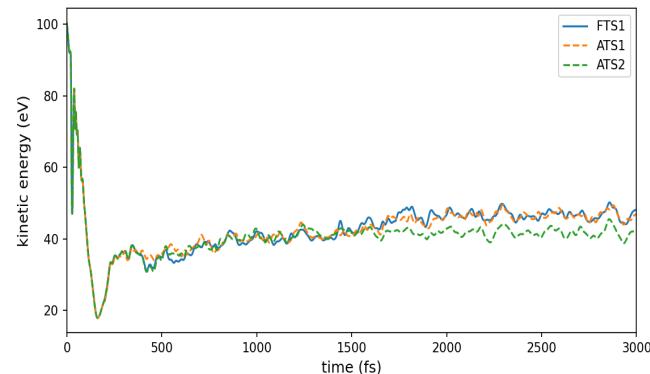
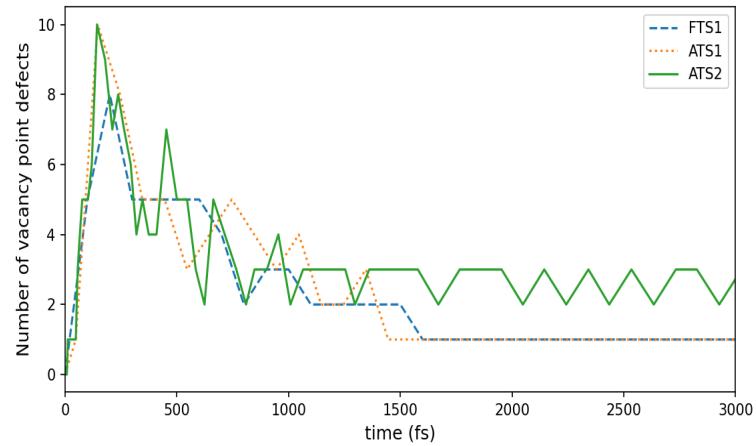
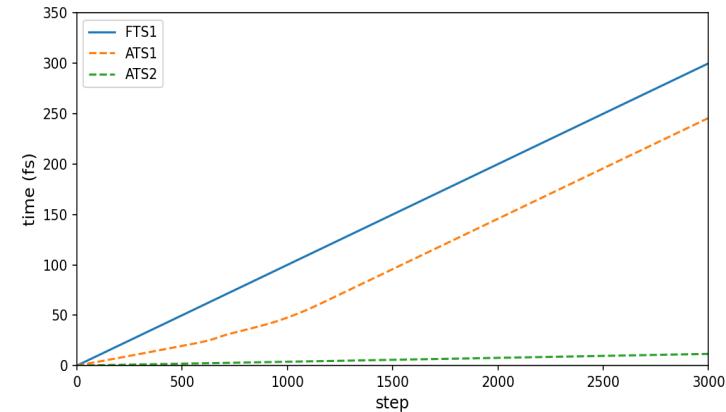
Fixed time step
= 0.1 fs → **FTS1**

ATS1

adapt_tstep_interval = 1
adapt_tmin = 1.0E-07
adapt_tmax = 1.0E-01
adapt_xmax = **1.0E-02**
adapt_emax = 30.0

ATS2

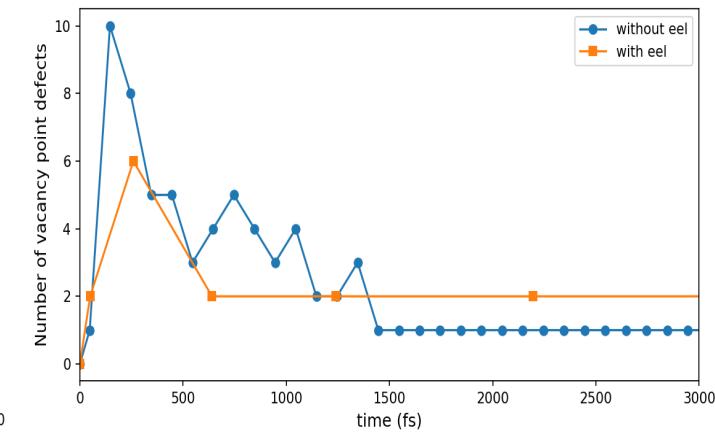
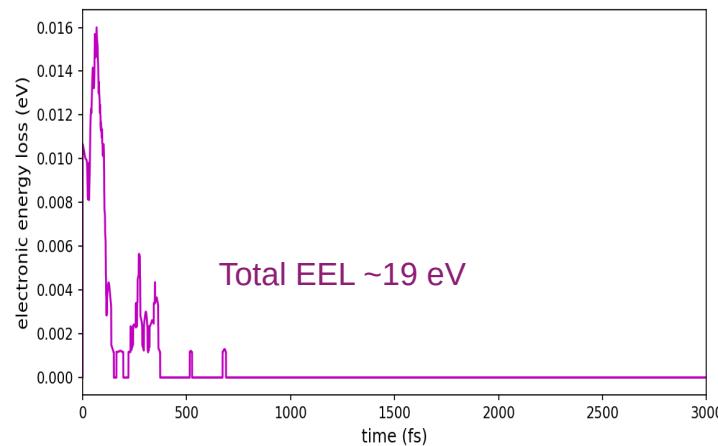
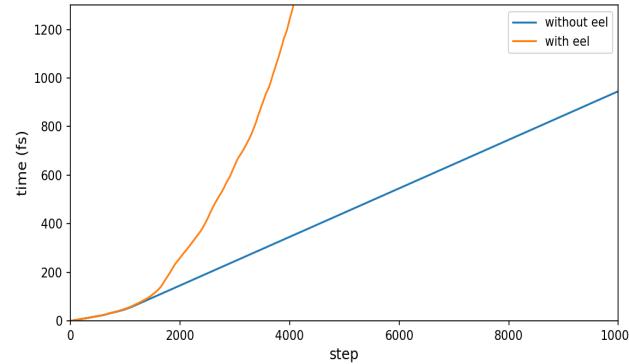
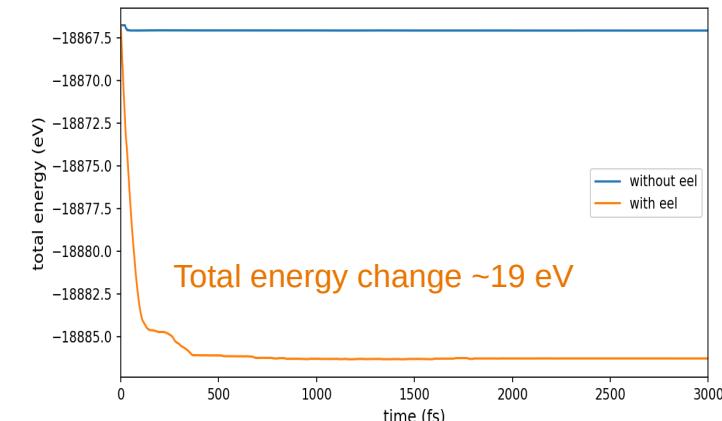
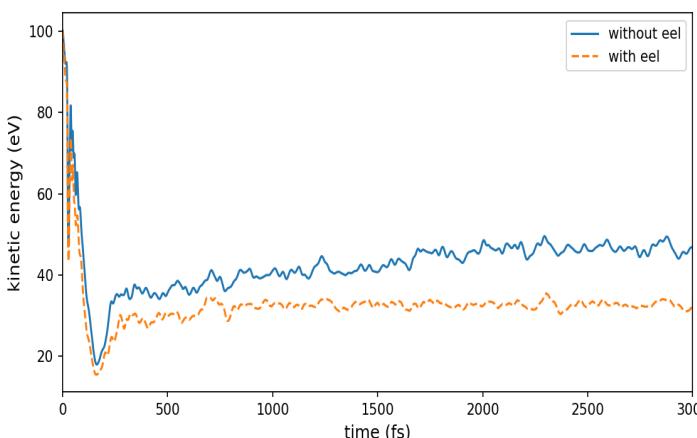
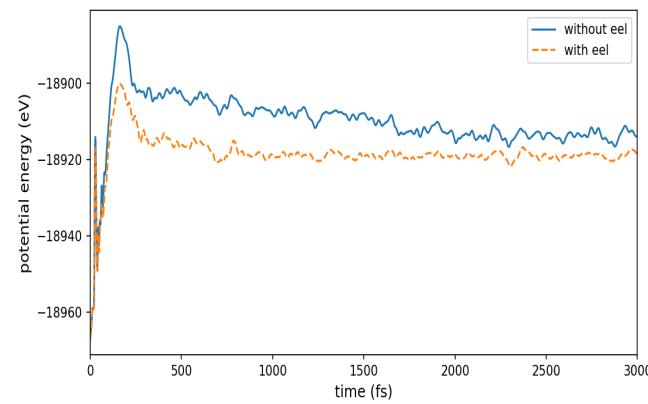
adapt_tstep_interval = 1
adapt_tmin = 1.0E-07
adapt_tmax = 1.0E-01
adapt_xmax = **1.0E-03**
adapt_emax = 30.0



Simulations with Electronic Stopping using stopping data from SRIM-2013

Silicon with 4096 atoms – one atom is given ~100 eV energy

eel_cut = 10.0 eV,
 tstep_interval = 1,
 tmin = 1.0E-07 fs, tmax = 1.0 fs,
 xmax = 0.01Å, emax = 30.0 eV



If we do not account EEL, then we allow more defect creation and also more defect annealing. The defects may also be morphologically different from reality. [Note: the numbers of defects or exact values of the quantities shown here are not important, only the general trends are shown by using a general purpose potential without short distance repulsive stiffening.]

Electronic stopping and electron-phonon coupling

During the initial non-equilibrium stages of a radiation event, electronic stopping is dominant and at the later stages to equilibrium between the lattice and the electrons, the coupling between electrons and lattice phonons become significant.

Both aspects of energy dissipation between the atoms and electrons are important.

The previous method described simply acts as a friction term

- to only reduce the energy of the atoms,
- to arbitrarily low values determined by the cut off energy specified and
- assumes that electronic stopping at low velocities is linear in velocity.

However,

- electronic stopping and e-ph coupling both must be accounted within same theory,
- a Langevin drag force can act between atoms and electronic heat bath establishing thermal equilibrium, not only just reducing the atom energy to arbitrary values,
- fixing the low energy cut off to arbitrary values may not be correct,
- at low velocities the electronic stopping power is not linear in velocity and
- the drag force connected to a stochastic force through fluctuation-dissipation theorem within the Langevin dynamical theory can model the phenomena more accurately.

The inputs to be given to implement this electron-phonon coupling model are described here. There are two choices:
<1> less input keywords with accompanying text file for electronic temperature mesh and
<2> using a few more input keywords, but no additional file.

Choice <1>

```
nonadiabatic_processes = .true.  
model_eph = 1  
eph_fdm_option = 1  
eph_friction_option = 1  
eph_random_option = 1  
eph_betafile = 'Si_PRB2021_constant.beta'  
eph_Tinfile = 'T_input.fdm'  
eph_md_last_step = 0  
eph_md_prev_time = 0.0  
eph_E_prev_time = 0.0  
eph_freq_Tout = 10  
eph_freq_mesh_Tout = 1000  
eph_Toutfile = 'T-Si-Ta0Te50.out'
```

For Choice <1> Sample T_input.fdm

```
#  
# 3 lines of comments  
#  
2 2 2 1  
0.0 16.29  
0.0 16.29  
0.0 16.29  
i j k T_e S_e rho_e C_e K_e flag T_dyn_flag  
1 1 1 50.0 1.0 1.0 3.5E-06 0.1248 0 0  
2 1 1 50.0 1.0 1.0 3.5E-06 0.1248 0 0  
1 2 1 50.0 1.0 1.0 3.5E-06 0.1248 0 0  
2 2 1 50.0 1.0 1.0 3.5E-06 0.1248 0 0  
1 1 2 50.0 1.0 1.0 3.5E-06 0.1248 0 0  
2 1 2 50.0 1.0 1.0 3.5E-06 0.1248 0 0  
1 2 2 50.0 1.0 1.0 3.5E-06 0.1248 0 0  
2 2 2 50.0 1.0 1.0 3.5E-06 0.1248 0 0
```

Choice <2>

```
nonadiabatic_processes = .true.  
model_eph = 1  
eph_fdm_option = 1  
eph_friction_option = 1  
eph_random_option = 1  
eph_betafile = 'Si_PRB2021_constant.beta'  
box_limits = 0.0 16.29 0.0 16.29 0.0 16.29  
eph_rho_e = 1.0  
eph_C_e = 3.5E-06  
eph_kappa_e = 0.1248  
eph_Ti_e = 50.0  
eph_gsx = 2  
eph_gsy = 2  
eph_gsz = 2  
eph_fdm_steps = 1  
eph_md_last_step = 0  
eph_md_prev_time = 0.0  
eph_E_prev_time = 0.0  
eph_freq_Tout = 10  
eph_freq_mesh_Tout = 1000  
eph_Toutfile = 'T-Si-Ta0Te50.out'
```

Some simulations by using the e-ph coupling model in TurboGAP are shown in the following few pages.

Variations of atomic and electronic temperatures

216 Si atoms in a box of dimensions
16.29 Å on each side.

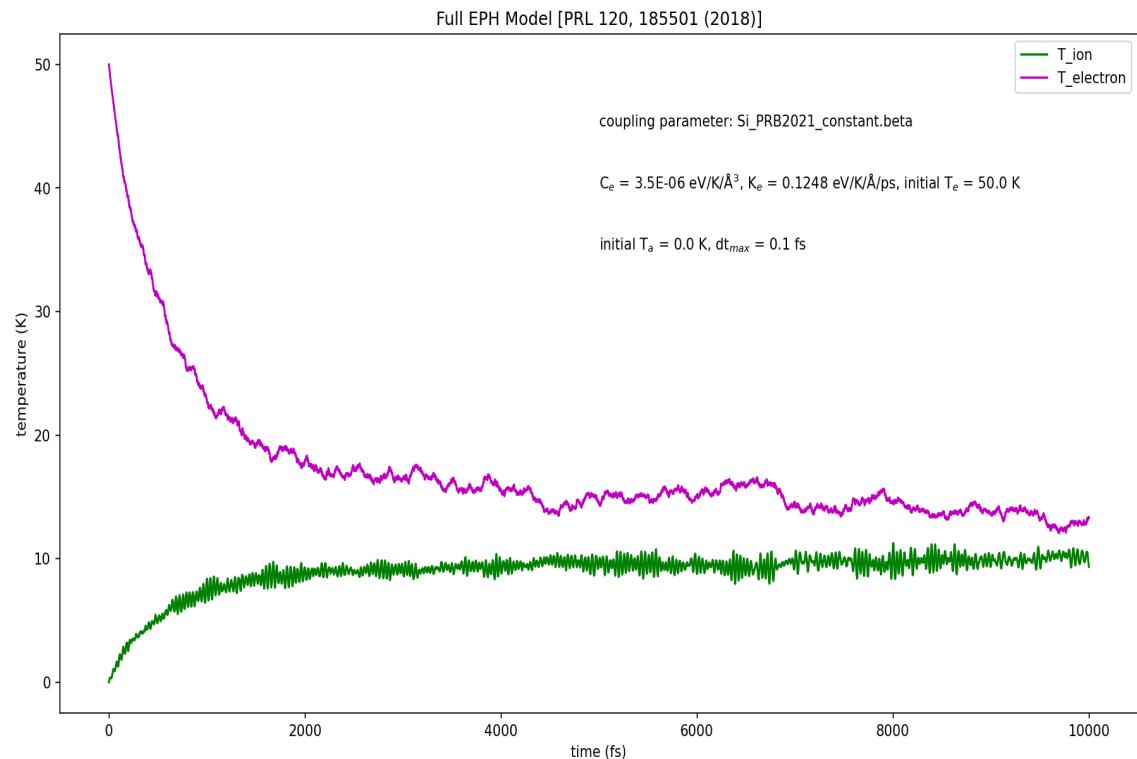
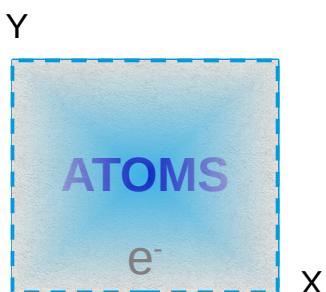
Initial atom temperature = 0.0 K

Initial electronic temperature = 50.0 K

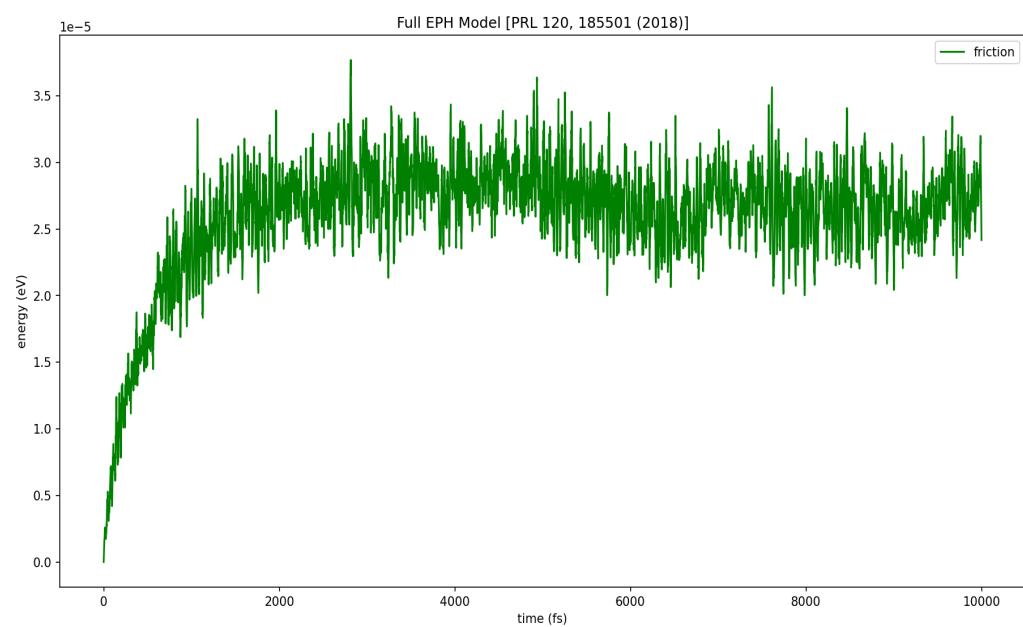
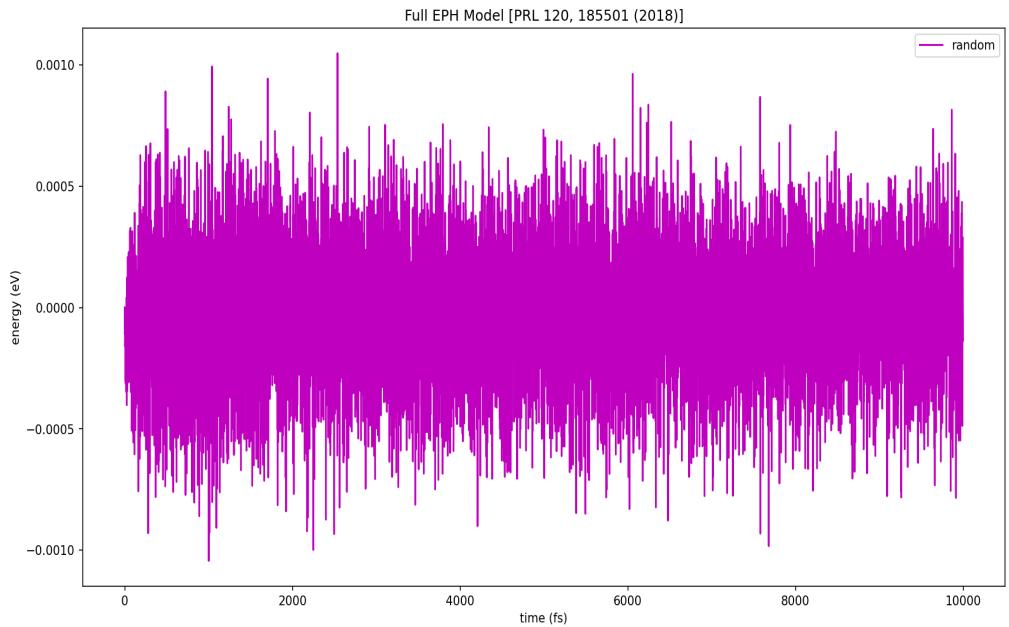
Coupling parameter – constant case
T. Jarrin et al. Phys. Rev. B 104, 195203

Electronic parameters:
 $C_e = 3.5 \times 10^{-6} \text{ eV/K/Å}^3$
 $K_e = 0.1248 \text{ eV/K/Å/ps}$

Electronic mesh:
Same size as atom box.
 $n_x = 1, n_y = 1, n_z = 1$.

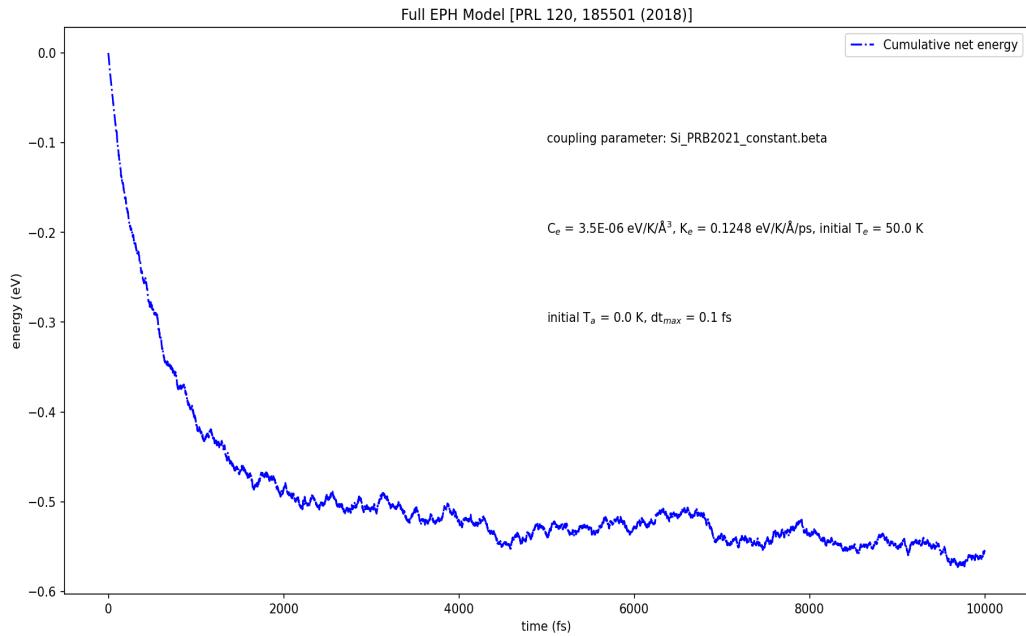


Variations of energies

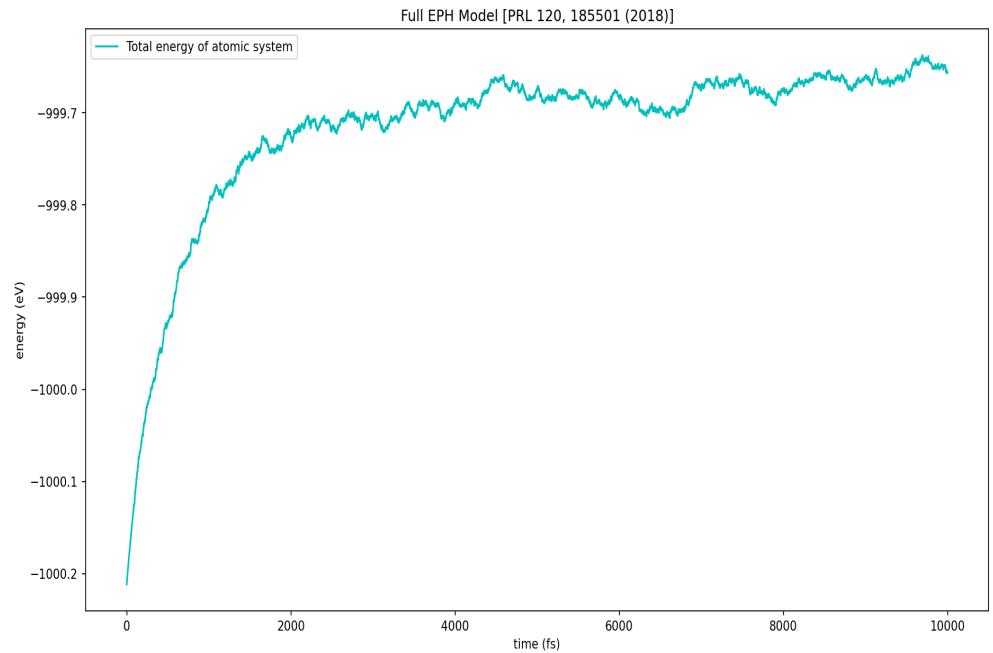


Variations of energies

Electronic system



Atomic system

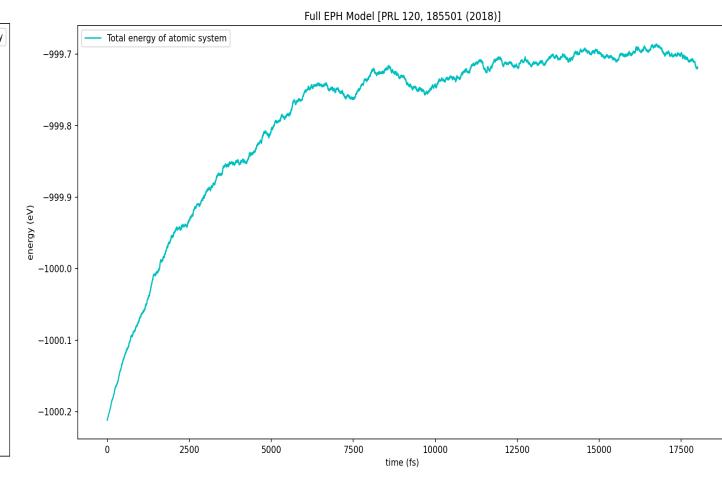
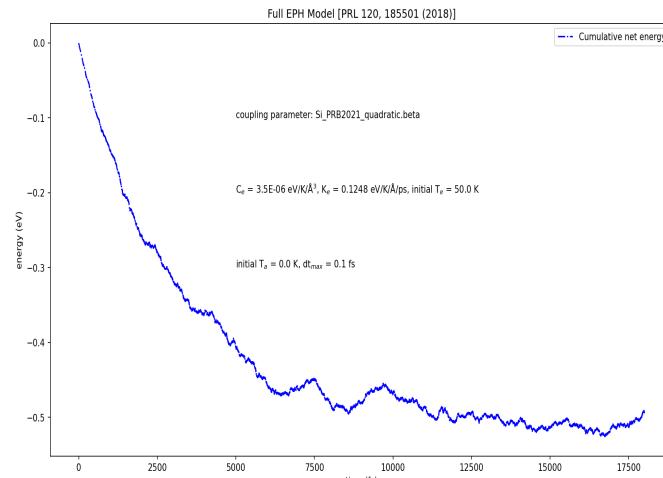
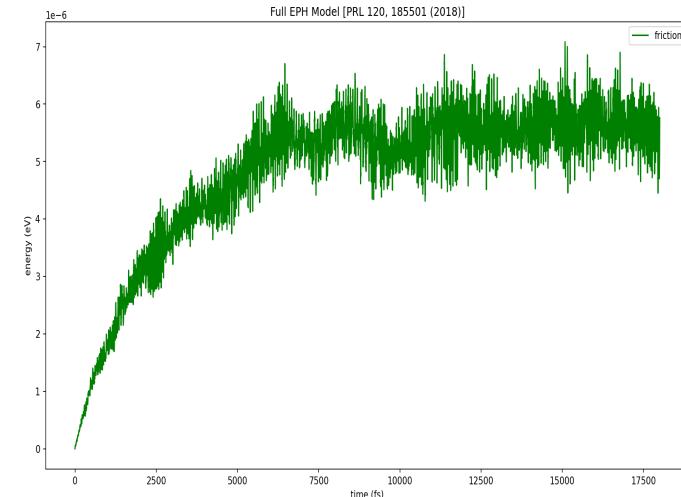
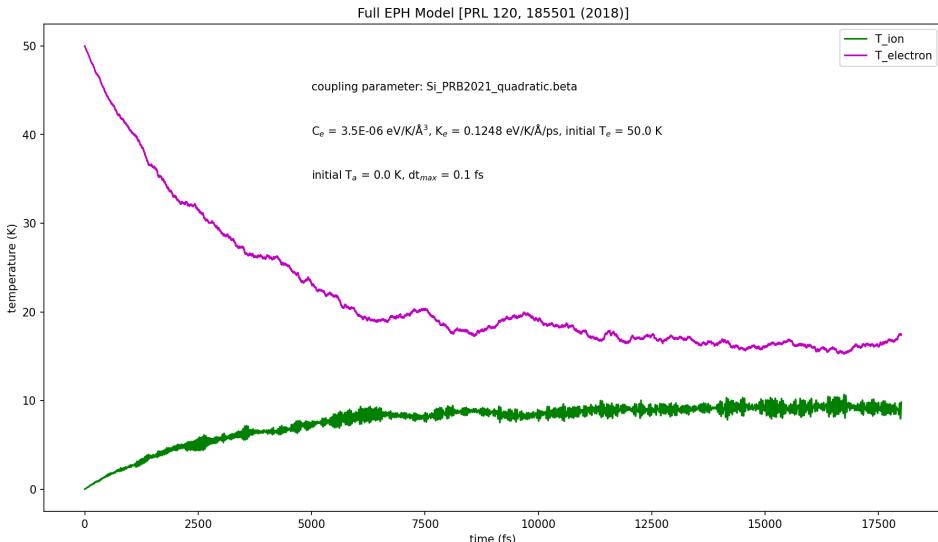


Energy is transferred from electronic to atomic system

Different coupling parameter will show some difference in rates to equilibrium.

There will also be some differences in the energies dissipated through friction and random forces

Coupling parameter – quadratic case T. Jarrin et al. Phys. Rev. B 104, 195203



Variations of atomic and electronic temperatures

The electronic mesh can be coarse or fine

216 Si atoms in a box of dimensions
16.29 Å on each side.

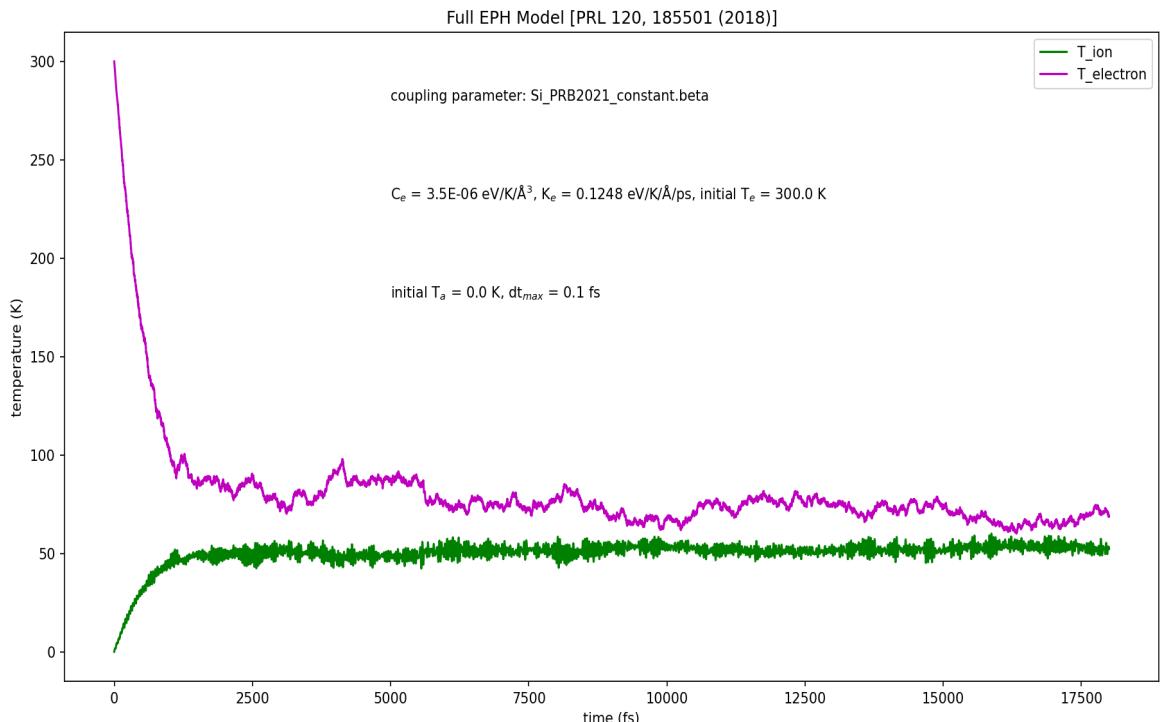
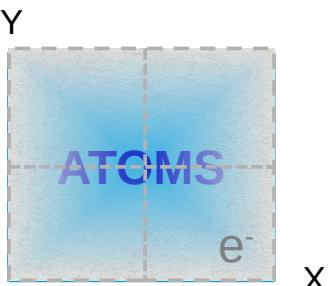
Initial atom temperature = 0.0 K

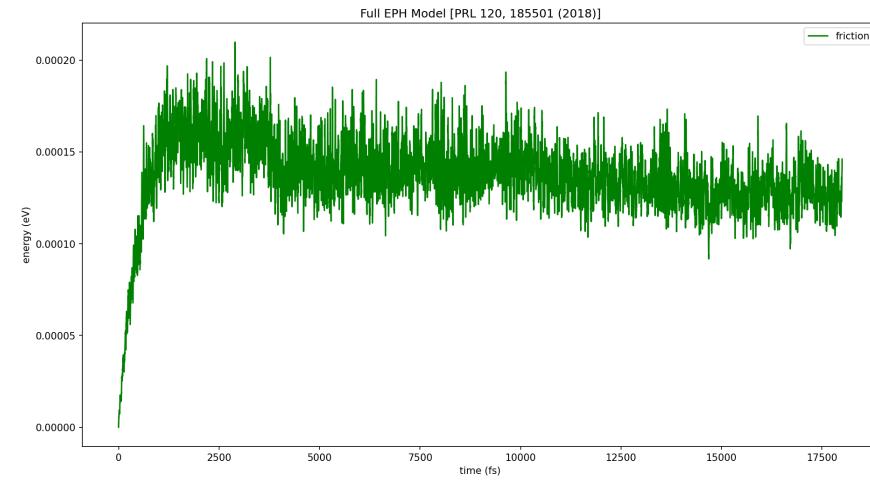
Initial electronic temperature = 300.0 K

Coupling parameter - constant case
T. Jarrin et al. Phys. Rev. B 104, 195203

Electronic parameters:
 $C_e = 3.5 \times 10^{-6} \text{ eV/K/Å}^3$
 $K_e = 0.1248 \text{ eV/K/Å/ps}$

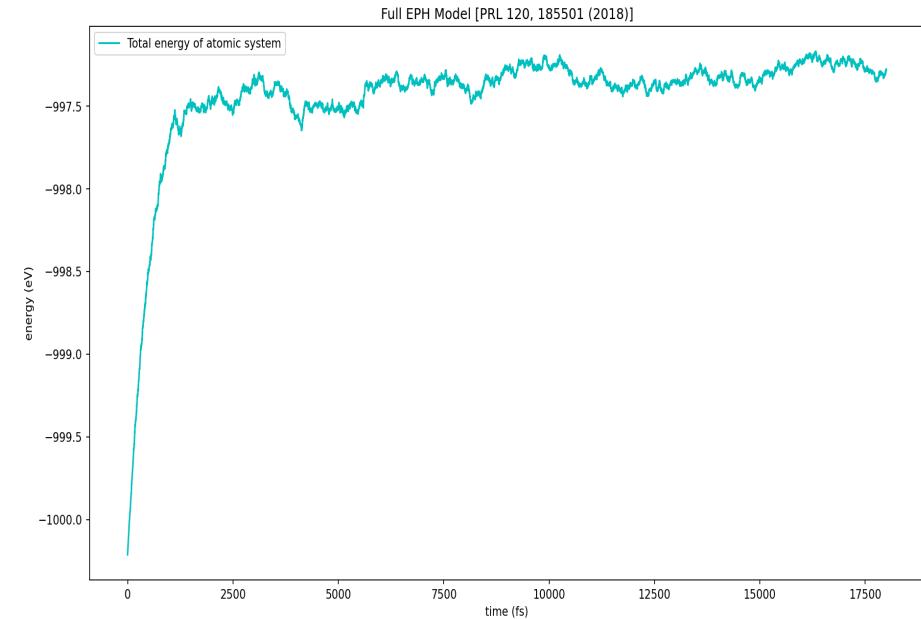
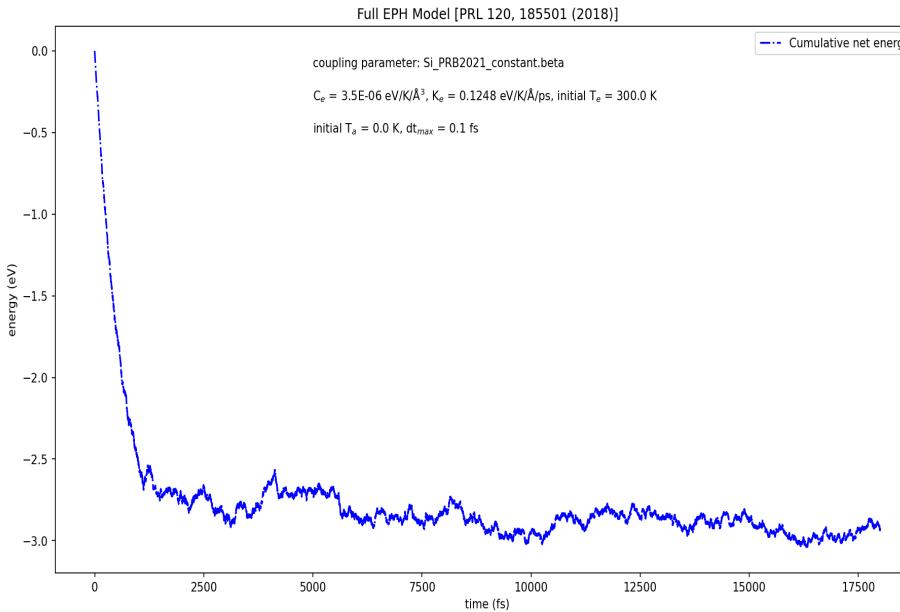
Electronic mesh:
Same size as atom box.
 $n_x = 2, n_y = 2, n_z = 2$.





Variations of energies

Energy is transferred from the electrons to the atoms



Along with the Coupling parameter, Electronic parameters also have effect on the Temperatures at equilibrium and the Energies dissipated

216 Si atoms in a box of dimensions 16.29 Å on each side.

Initial atom temperature = 0.0 K

Initial electronic temperature = 50.0 K

Coupling parameter – constant case
T. Jarrin et al. Phys. Rev. B 104, 195203

Electronic parameters:

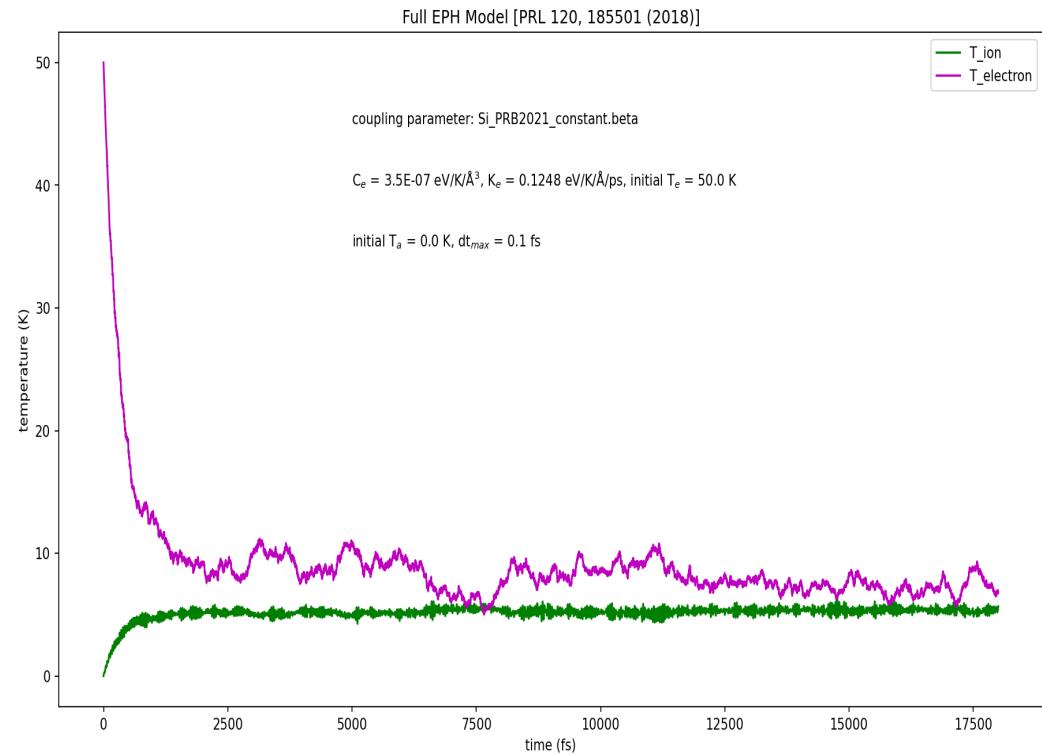
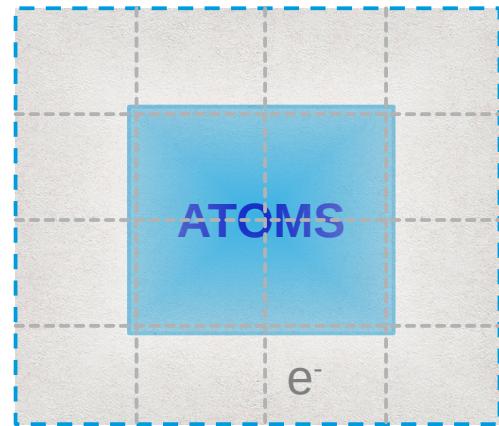
$C_e = 3.5 \times 10^{-7} \text{ eV/K/Å}^3$

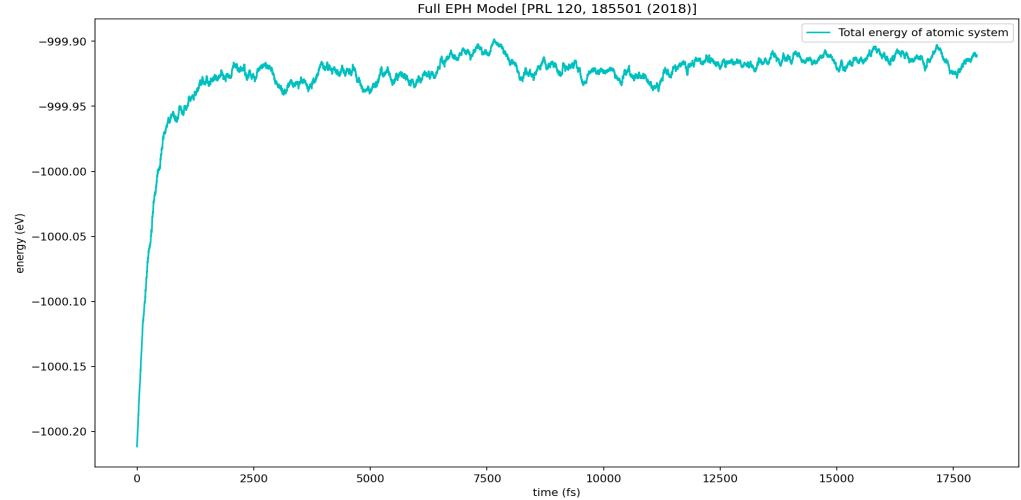
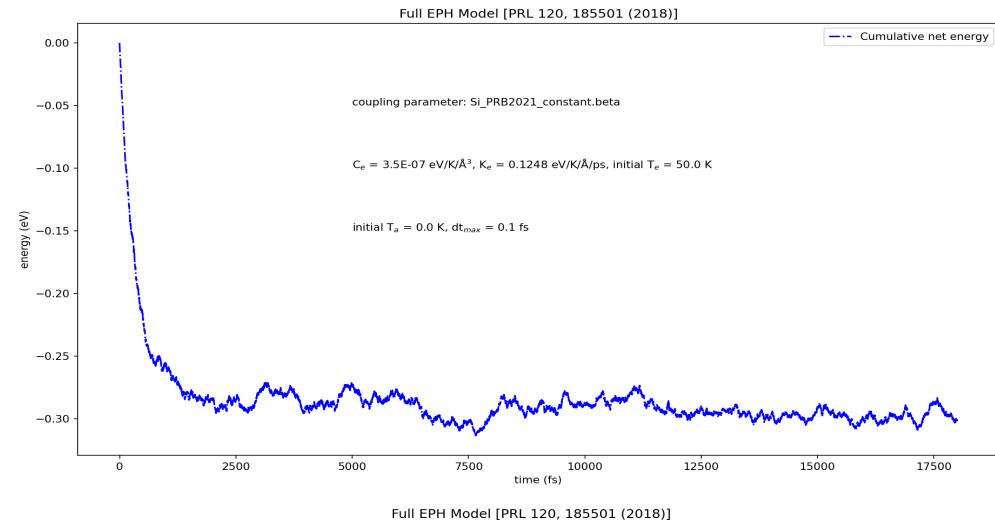
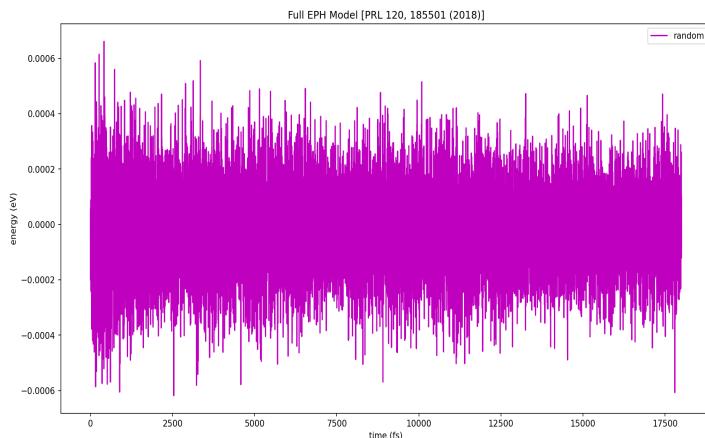
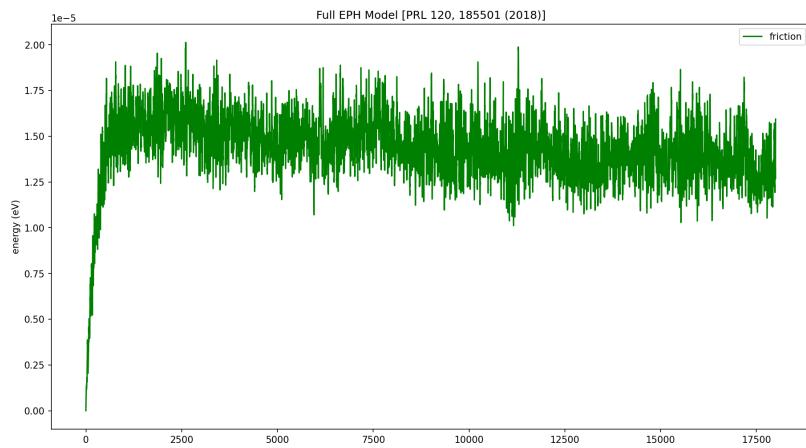
$K_e = 0.1248 \text{ eV/K/Å/ps}$

Electronic mesh:

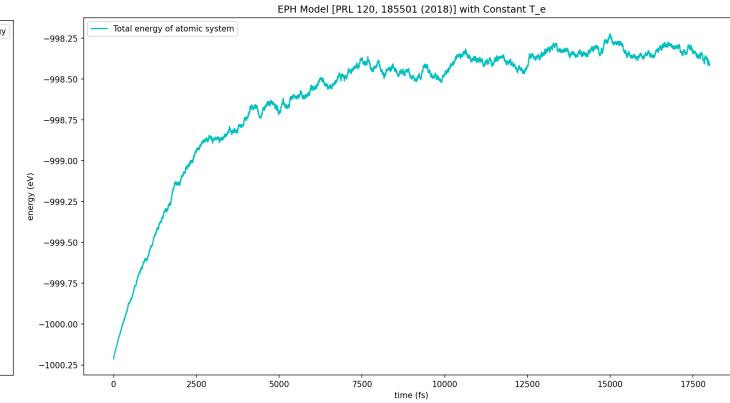
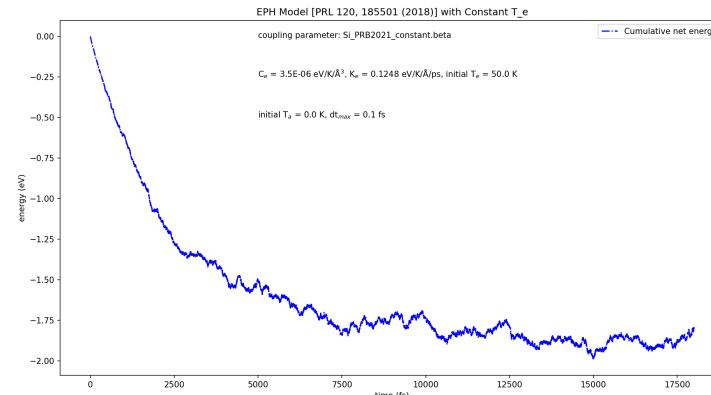
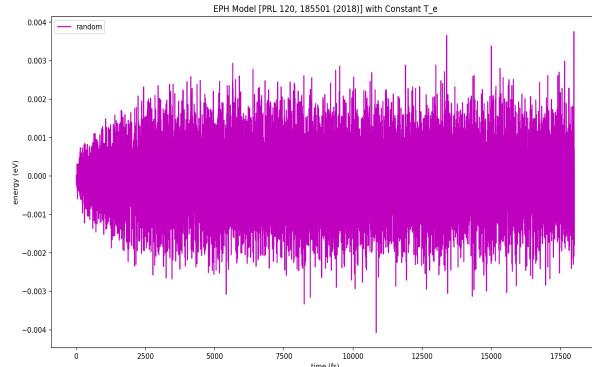
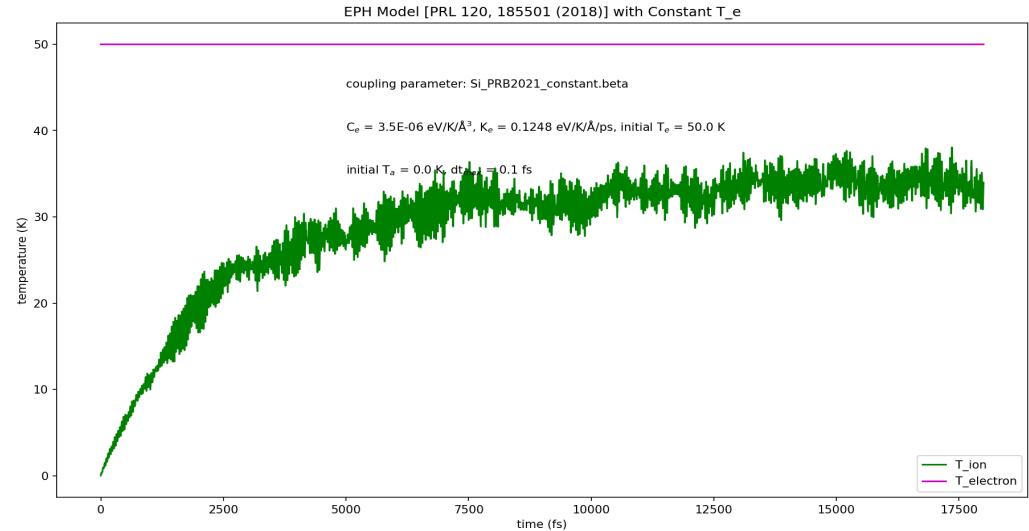
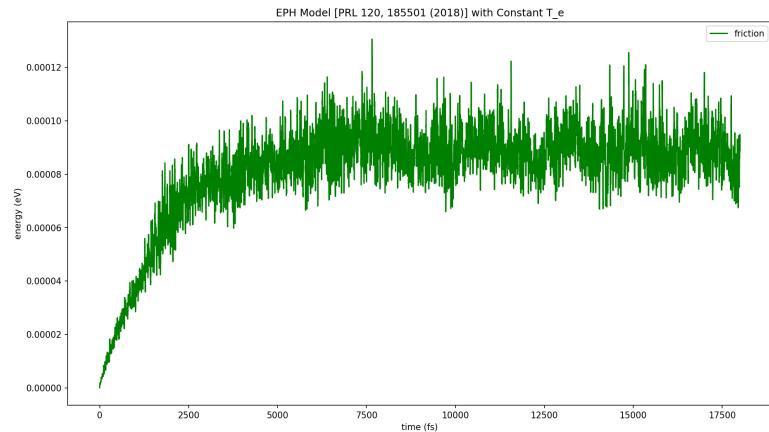
Larger than atom box
(-17.0 to +17.0 on each side).

$nx = 4, ny = 4, nz = 4$.

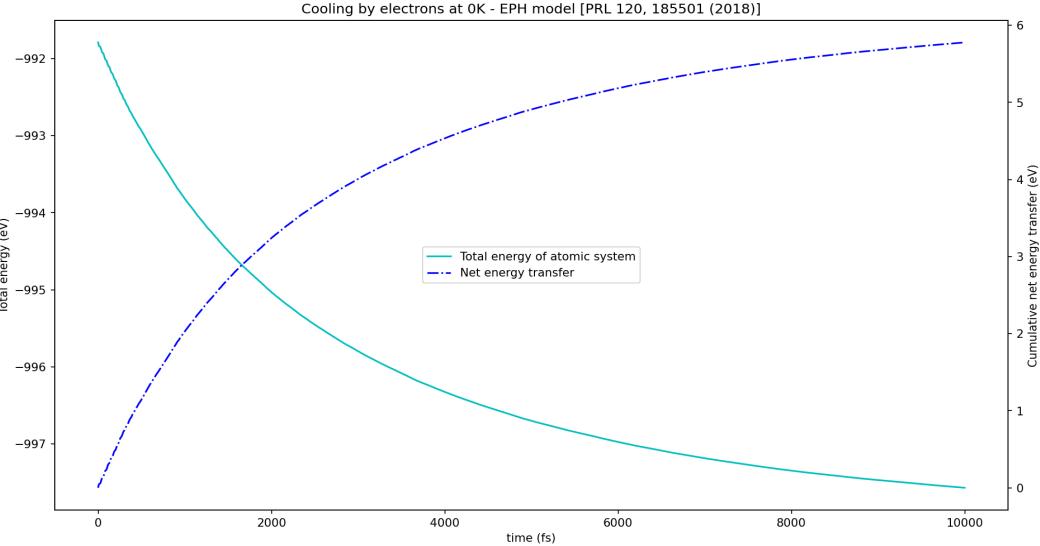
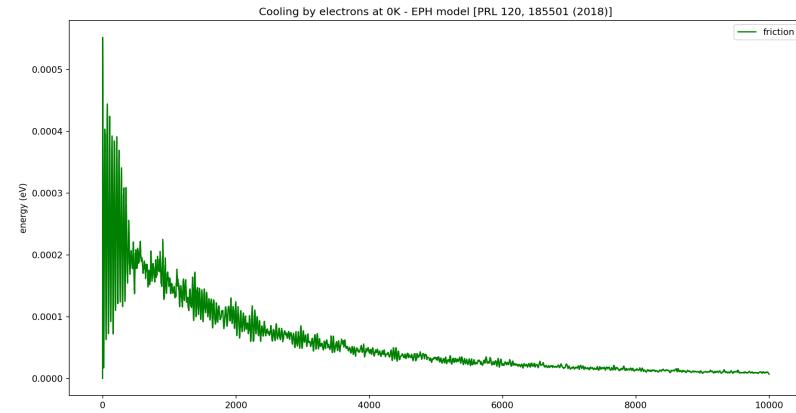
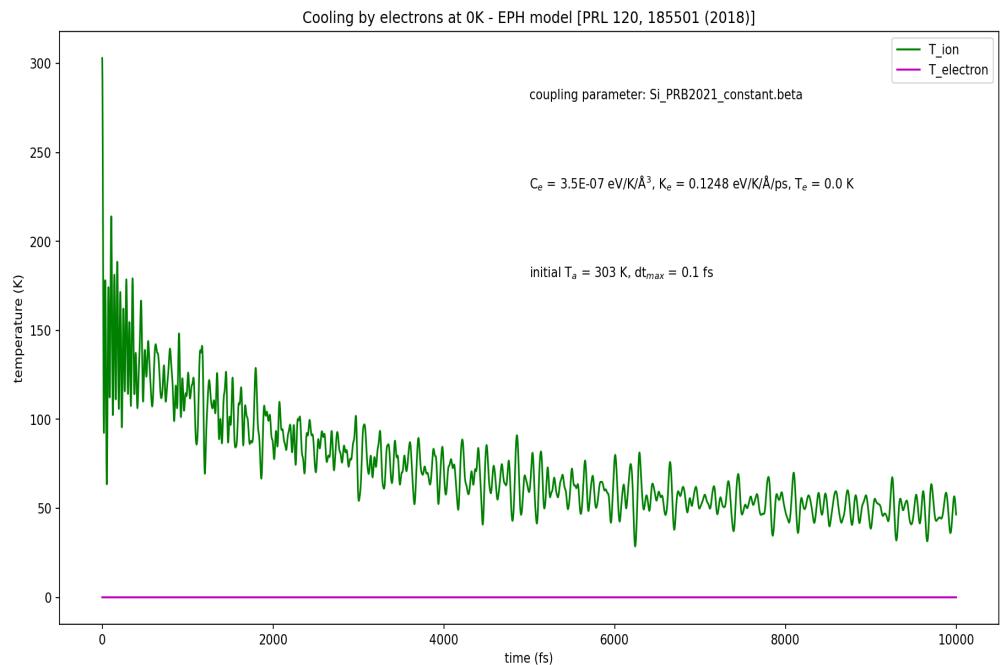




The electronic temperature is kept constant at 50 K and not updated



The system is cooled by friction forces only when the electrons are held at 0 K temperature



TurboGAP Simulations of 0.1 keV PKA with the EPH Model

EPH Model using Only Friction with 0.1 keV PKA

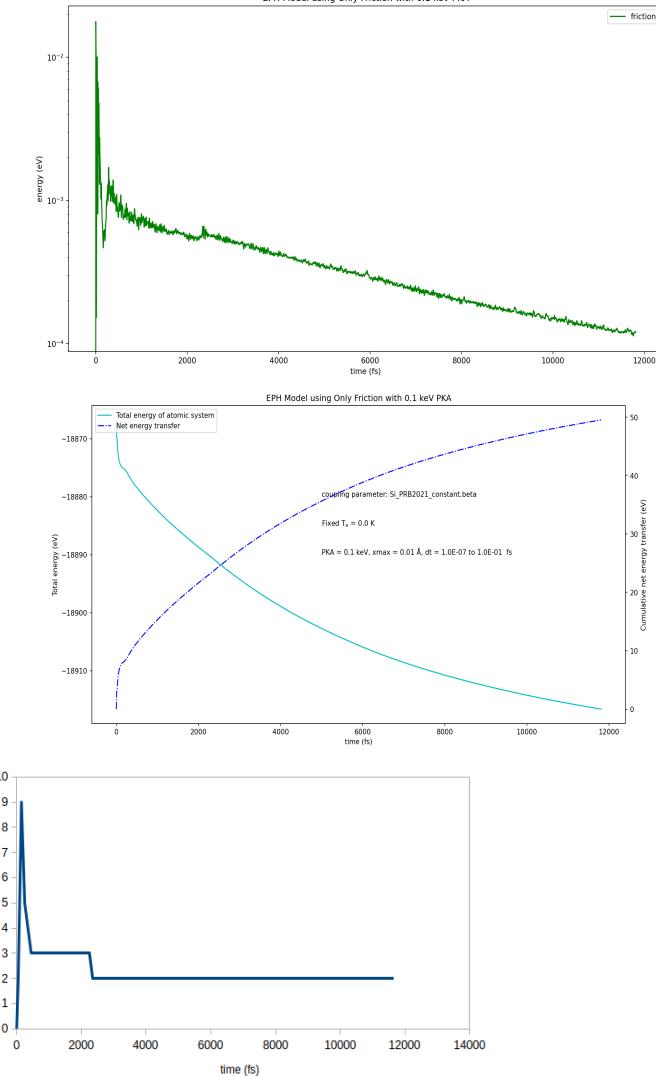
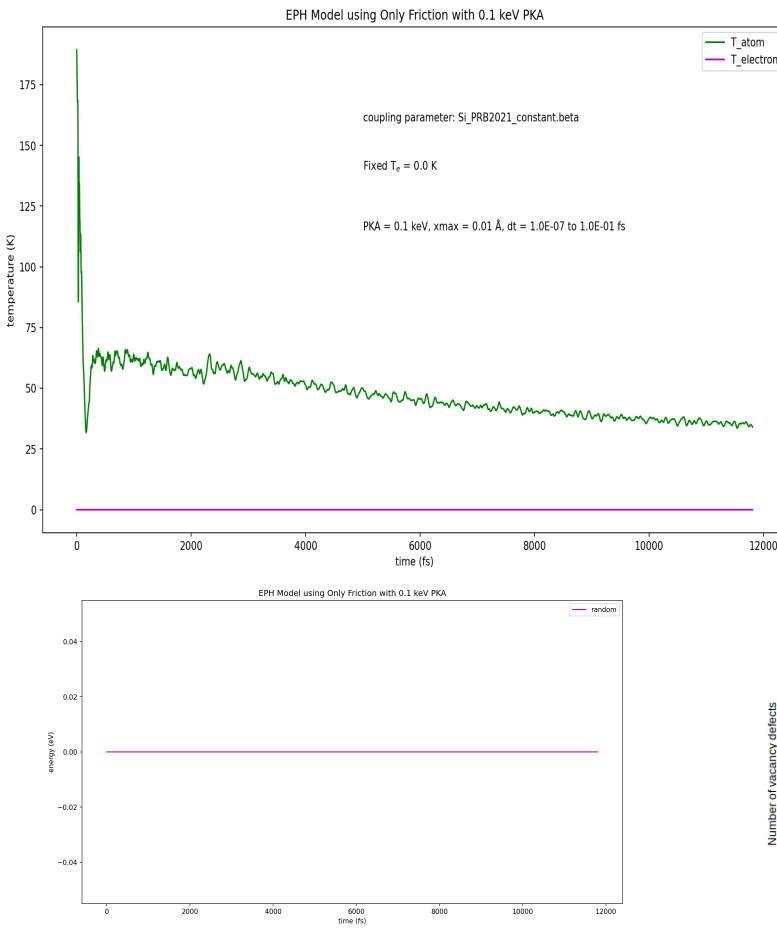
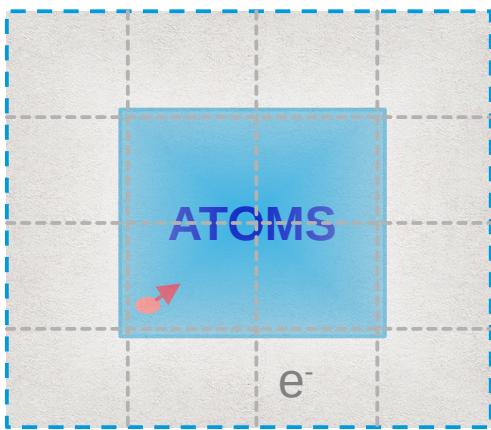
Only friction forces are applied

4096 Si atoms in a box of dimensions 43.44 \AA on each side.

Initial atom temperature $\sim 190 \text{ K}$ due to a 0.1 keV PKA

Initial and fixed electronic temperature = 0.0 K

Coupling parameter – constant case
T. Jarrin et al. Phys. Rev. B 104, 195203



TurboGAP Simulations of 0.1 keV PKA with the EPH Model

4096 Si atoms in a box of dimensions 43.44 Å on each side.

Initial atom temperature ~ 190 K due to a 0.1 keV PKA

Initial electronic temperature = 0.0 K

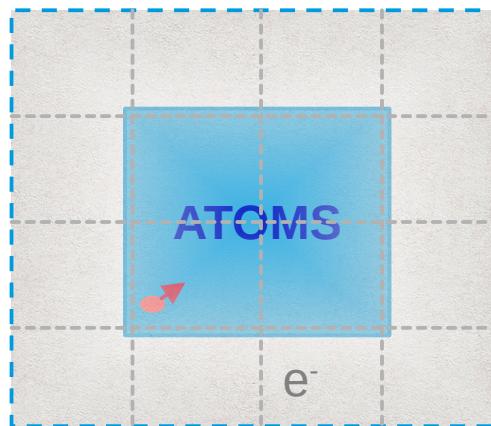
Coupling parameter – constant case
T. Jarrin et al. Phys. Rev. B 104, 195203

Electronic parameters:
 $C_e = 3.5 \times 10^{-6} \text{ eV/K/Å}^3$
 $K_e = 0.1248 \text{ eV/K/Å/ps}$

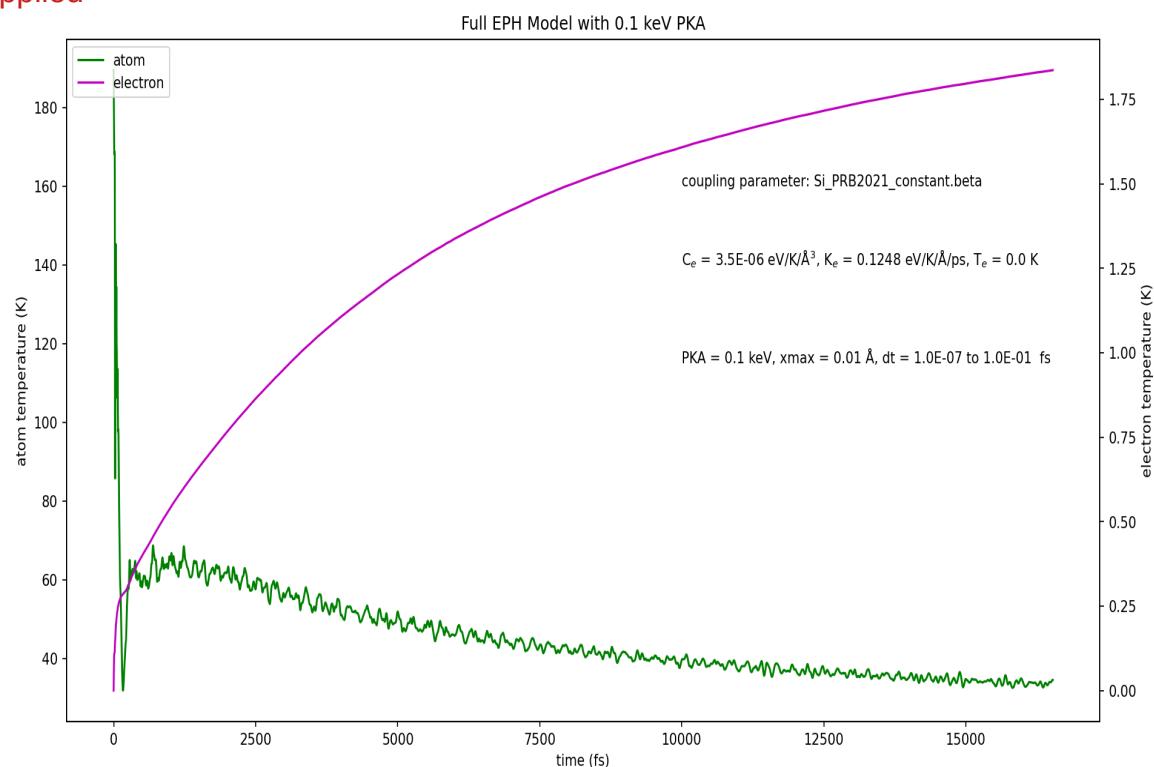
Electronic mesh:

Larger than atom box
(-100.0 to +100.0 on each side).

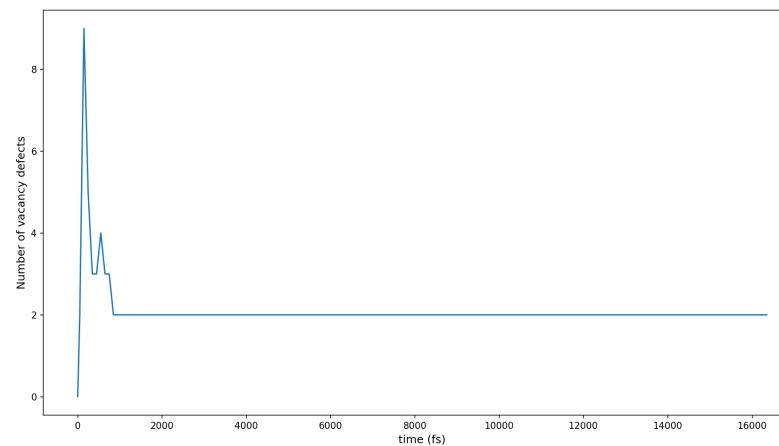
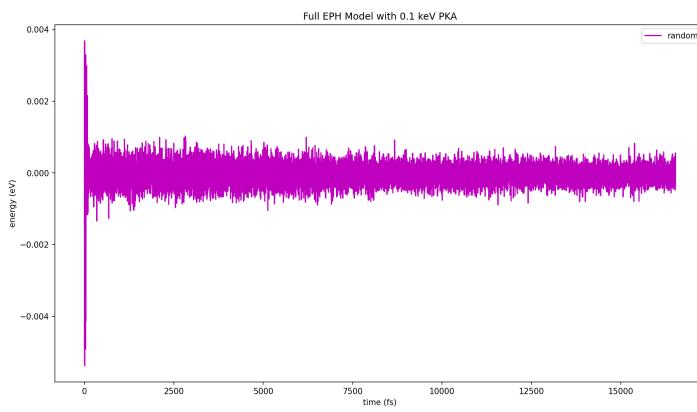
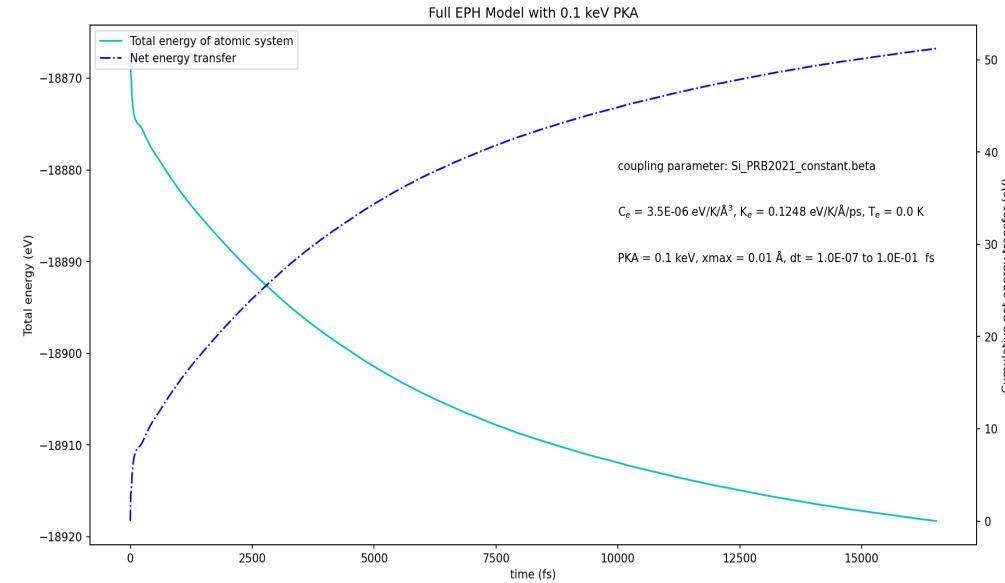
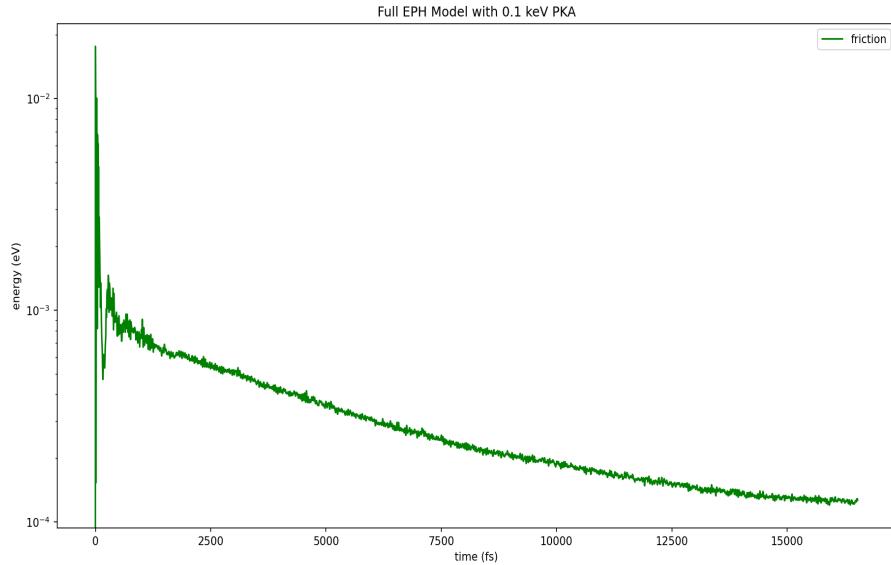
$nx = 4, ny = 4, nz = 4$.



Full model is applied



TurboGAP Simulations of 0.1 keV PKA with the EPH Model



Acknowledgements

Prof. Andrea Sand, Prof. Artur Tamm and Dr. Miguel A. Caro for good discussions.

Dr. Ali Hamedani for providing important feedback on adaptive time simulations with high energy knock-on atoms using repulsive GAP potentials.

The computational resources provided by the Aalto Science-IT project.