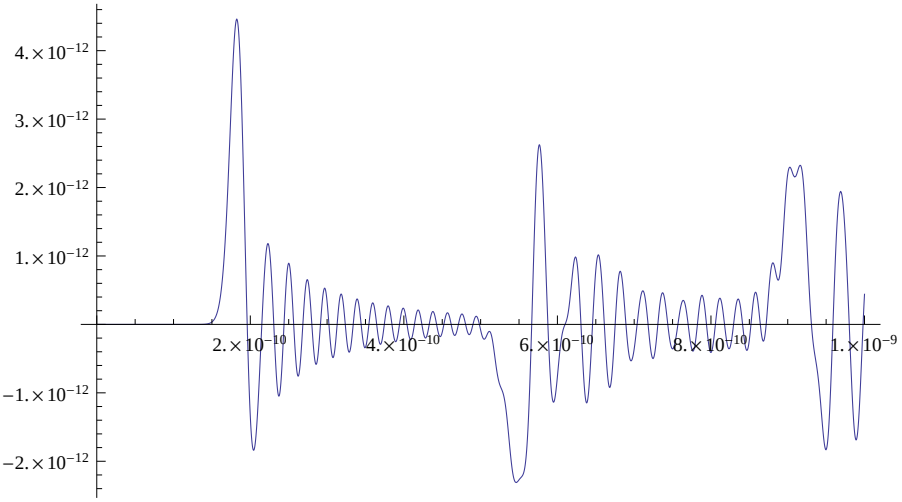
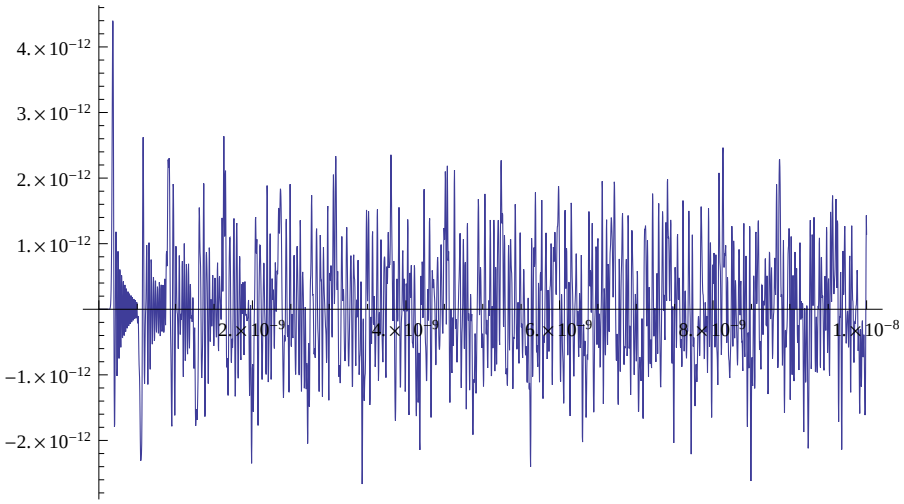
```
Avagadro = 6.022142 * 10^23;
ze = 2.42 * 10^-10; (*bond distance 2.42 A in m *)
Ebond = 300; (*bond Energy 300 kJ/mol *)
κ = 2.55 * 10^10; (*decay factor in 1/angstrom*)
m1 = 12 / Avagadro; (* weight of One Carbon Atom *)
IVel = 1; (* Initial Velocity of 1DOF model *)
IPos = ze; (*Initial Position of 1DOF atom *)
endtime = N[10^-8]; (*Simulation End Time*)

(*Formulas And Calculations*)
L = -Ebond * (2 * (ze / z)^6 - (ze / z)^12);
V = -Ebond * (2 * Exp[-κ * z] - Exp[-2 * κ * z]);
(*V=z^2/2;   For test Purposes*)
Va = V / Avagadro;
Fm = D[V, z] / Avagadro;

n = 32; (*lattice atoms*)
IPos = ConstantArray[0, n];
IVel = ConstantArray[0, n]; (*Initial Position of 1DOF atom *)
IVel[[n]] = 1;

Z = Table[ToExpression[StringJoin["z", ToString[i], "[t]"]], {i, 1, n}];

CarbonAtomWeight = N[12 / Avagadro];
OxygenAtomWeight = N[16 / Avagadro];

MArray = Table[CarbonAtomWeight, {i, 1, n}];
M = DiagonalMatrix[MArray];

VPotTemp = Total[Table[Va /. z → (Z[[i]] - Z[[i + 1]]), {i, 1, n - 1}]];
VPot = (Va /. z → Z[[1]]) + VPotTemp;


TKin = Sum[0.5 * M[[i, i]] * D[Z[[i]], t]^2, {i, 1, n}];
Lagrange = TKin - VPot ;

temp1 = Table[D[Lagrange, D[Z[[i]], t], t] - D[Lagrange, Z[[i]] ] == 0, {i, 1, n}];
temp2 =
  Table[{(Z[[i]] /. t → 0) == IPos[[i]], (D[Z[[i]], t] /. t → 0) == IVel[[i]]}, {i, 1, n}];

Eqs = Flatten[{temp1, temp2}];


solMDOF =
  NDSolve[Eqs, Z, {t, 0, endtime}, MaxSteps → ∞, PrecisionGoal → 13, AccuracyGoal → 13];
Plot[Evaluate[Z[[1]] /. solMDOF], {t, 0, endtime}, PlotRange → All,
  PlotLabel → "Atomic Displacements", ImageSize → 420]
 Plot[Evaluate[Z[[1]] /. solMDOF], {t, 0, endtime / 10}, PlotRange → All,
  PlotLabel → "Atomic Displacements", ImageSize → 420]
Plot[Evaluate[Z[[n]] /. solMDOF], {t, 0, endtime / 10}, PlotRange → All,
 PlotLabel → "Atomic Displacements", ImageSize → 420]
Plot[Evaluate[Z /. solMDOF], {t, 0, endtime / 10}, PlotRange → All,
 PlotLabel → "Atomic Displacements", ImageSize → 420]
```

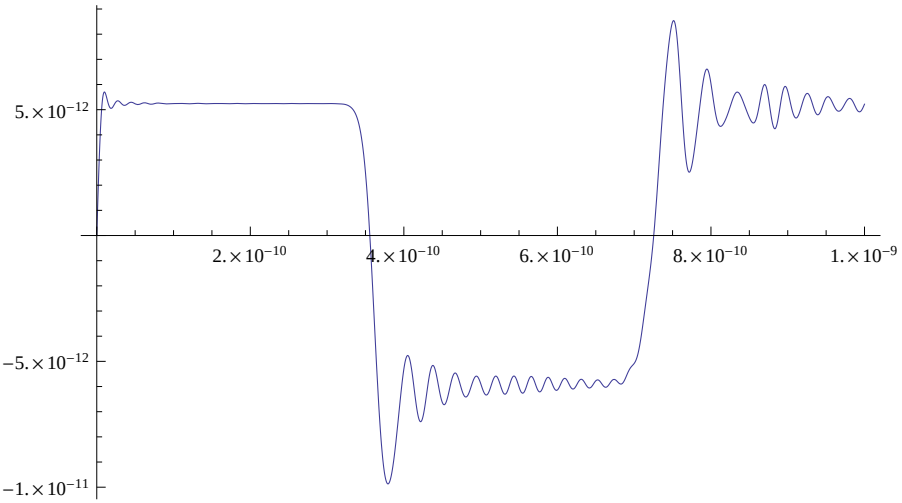
Atomic Displacements

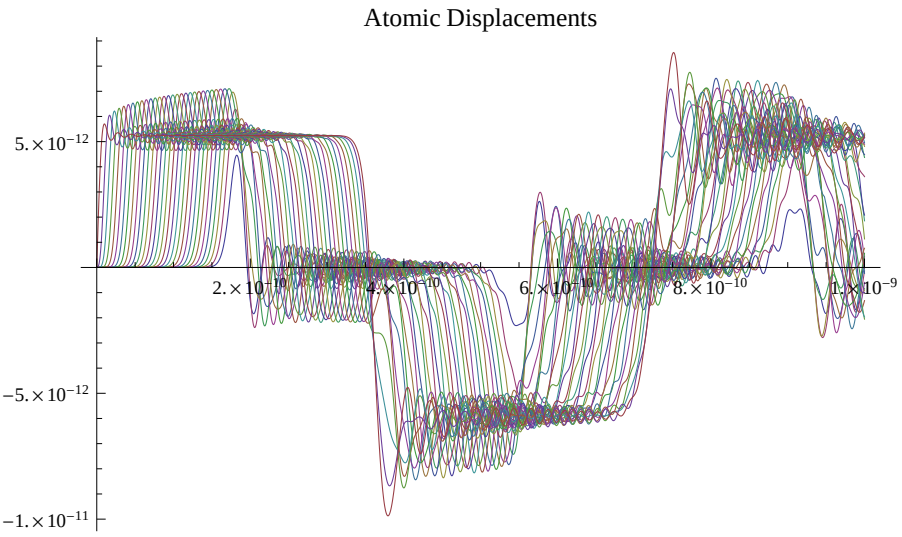


Atomic Displacements



Atomic Displacements




Atomic Displacements
5.×10^-12
-5.×10^-12
-1.×10^-11
2.×10^-10
4.×10^-10
6.×10^-10
8.×10^-10
1.×10^-9