Indium crystal melting – Molecular Dynamics Simulation

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TODAY'S DATE – 07/25/2016

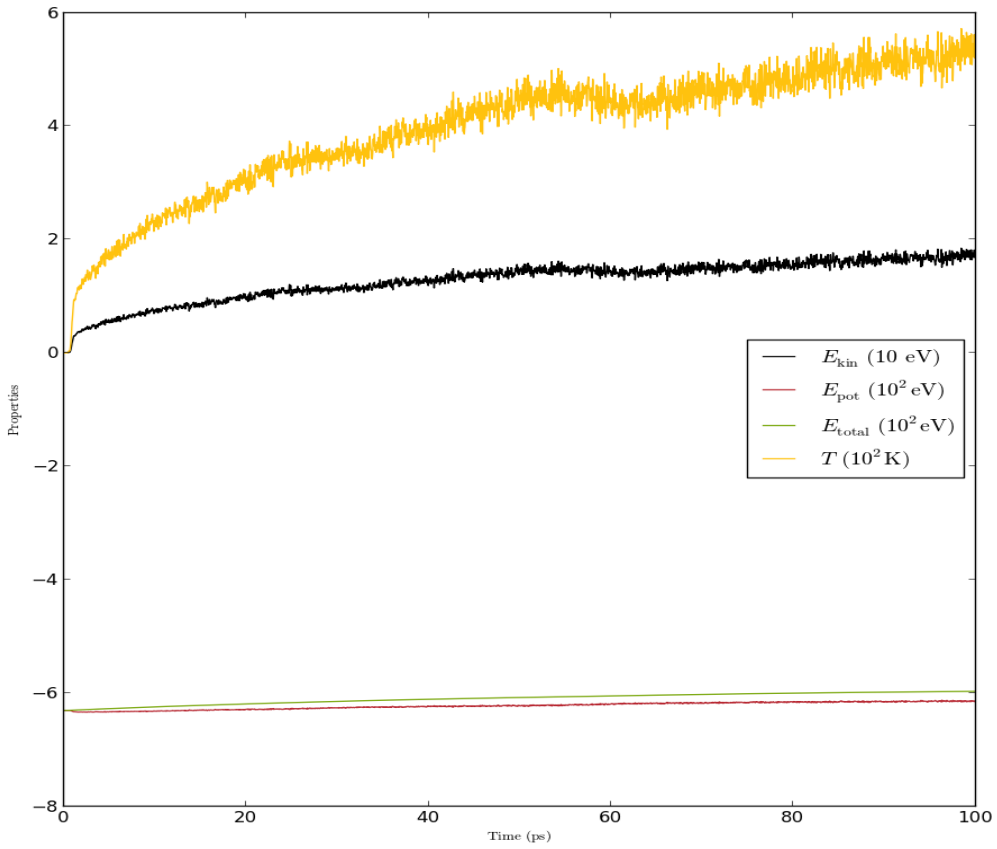
Activities this week

- Worked on simulating pure Indium melting phenomenon with QuantumWise.
- NPT Berendsen type MD was used throughout.
- Tersoff_InAs_2008 defined interatomic potential used in simulations.
- Significant output were those corresponding to 5x5x5 and 10x10x10 crystal structures.
- Plot corresponding to 5x5x5 Indium structure was very noisy whereas that corresponding to 10x10x10 was smoother.
- Both these cases indicated melting points near the expected 440 K.

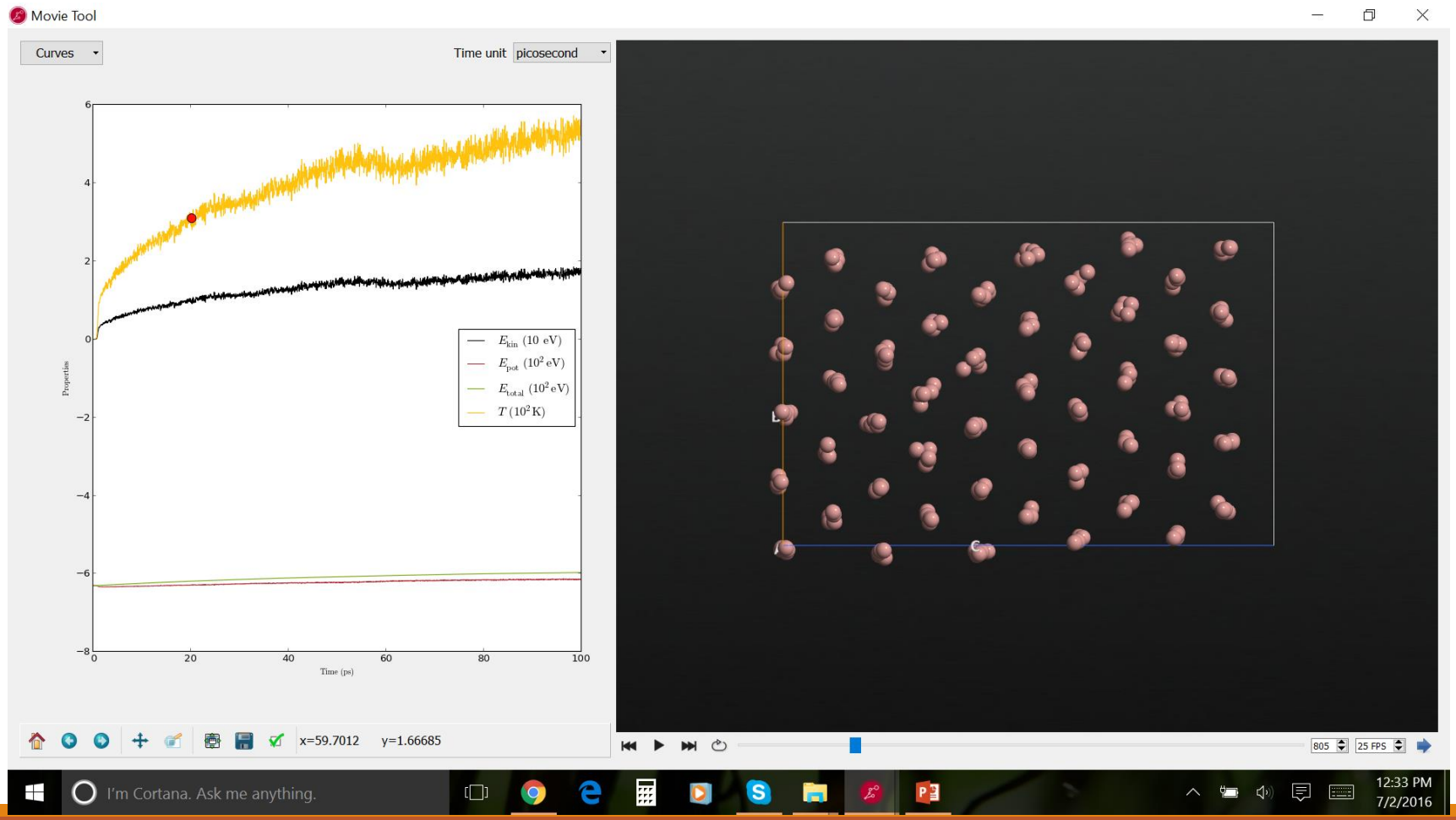
5x5x5 Indium structure

- Temp coupling – 30000 fs
- Press coupling – 25 fs
- Reservoir Temp – 800 K
- Maxwell Boltzmann initial vel.

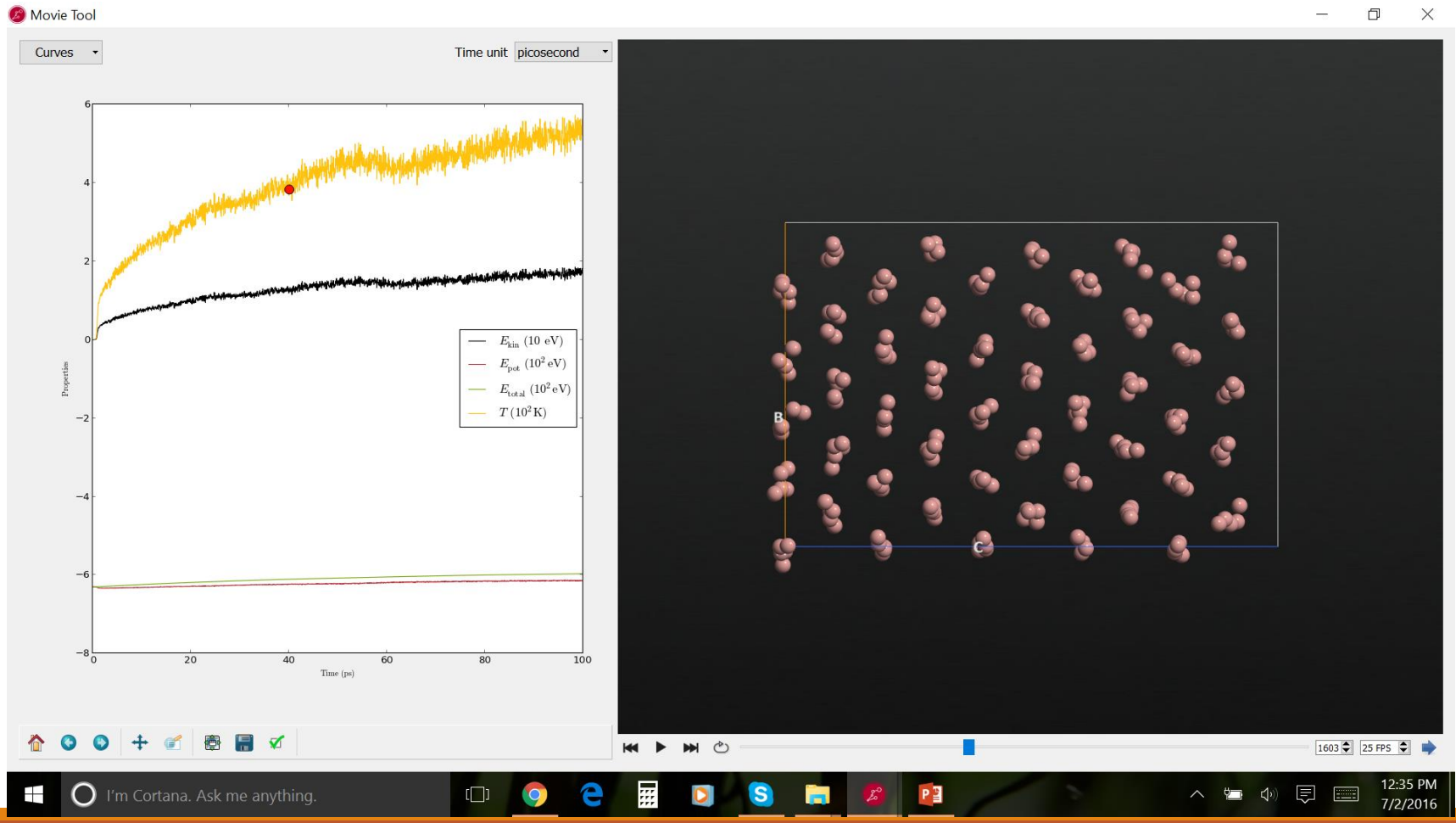
  Initial temp – 0 K
- Simulation steps – 100,000
- Indicated Melting point – 435 K



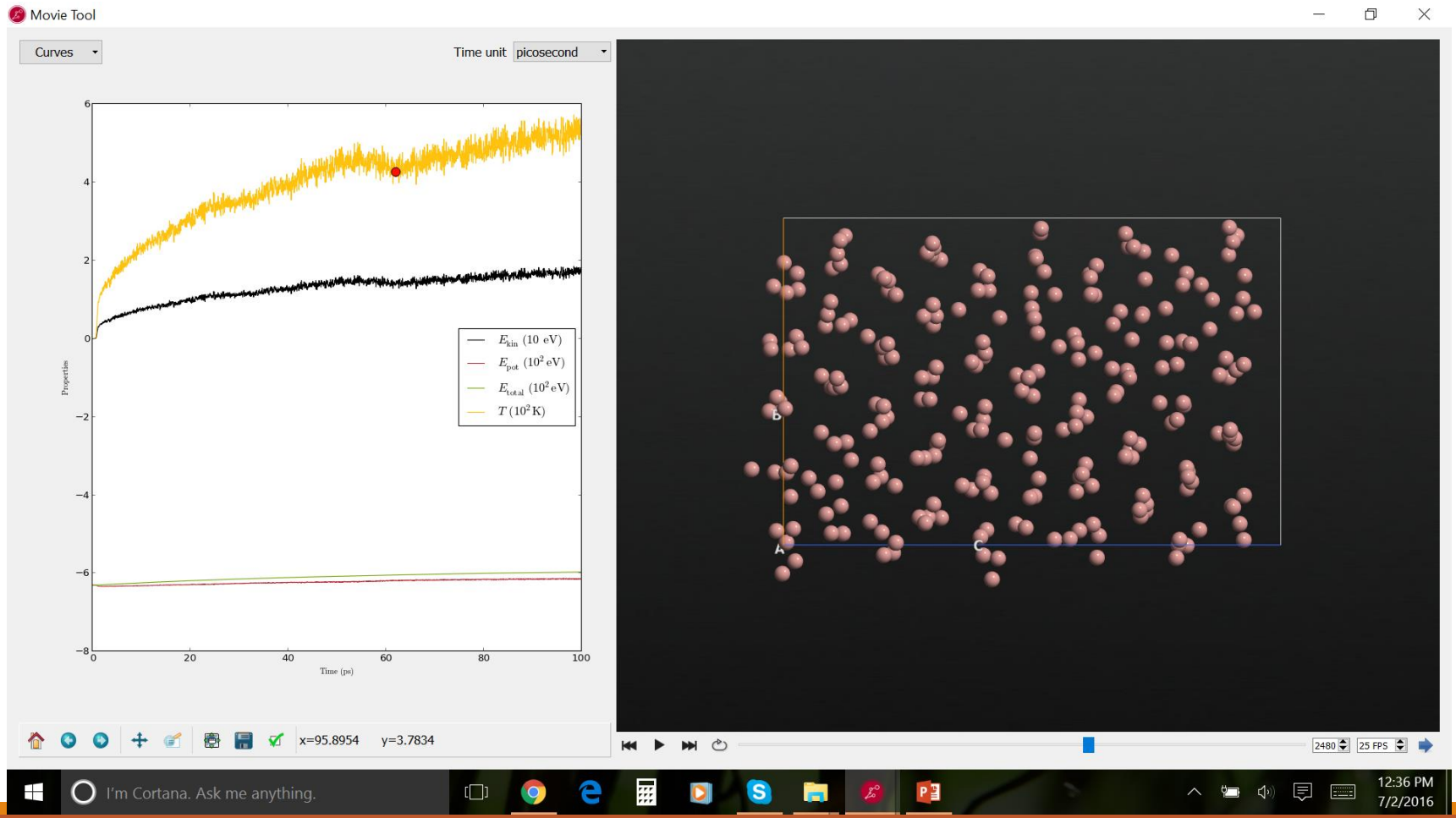
5x5x5 Indium melting – 20ps



5x5x5 Indium melting – 40ps

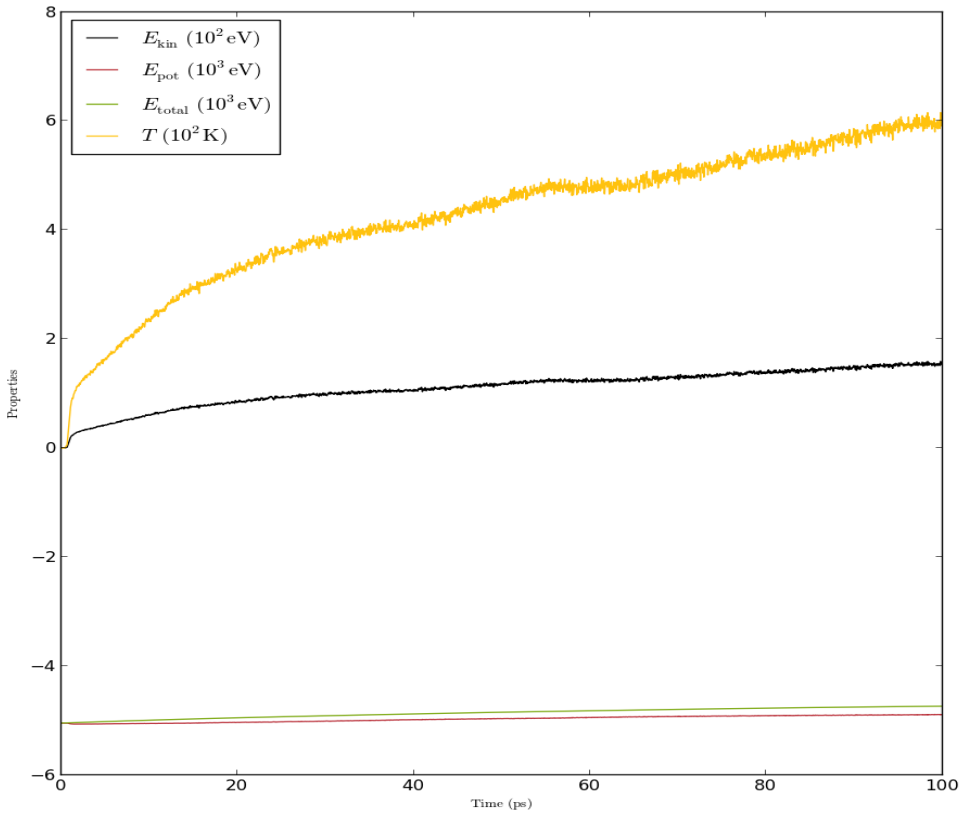


5x5x5 Indium – melting point

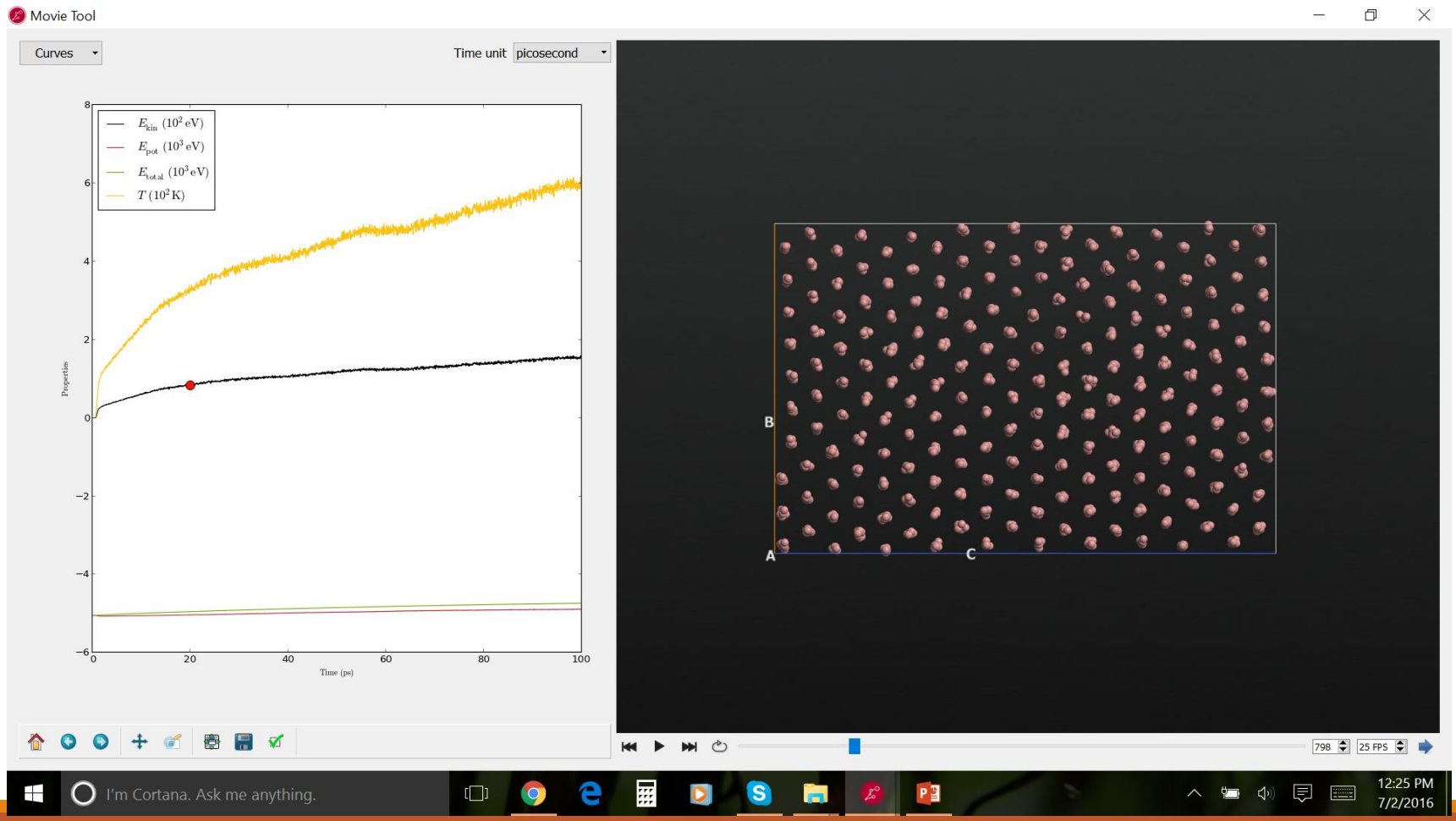


10x10x10 Indium structure

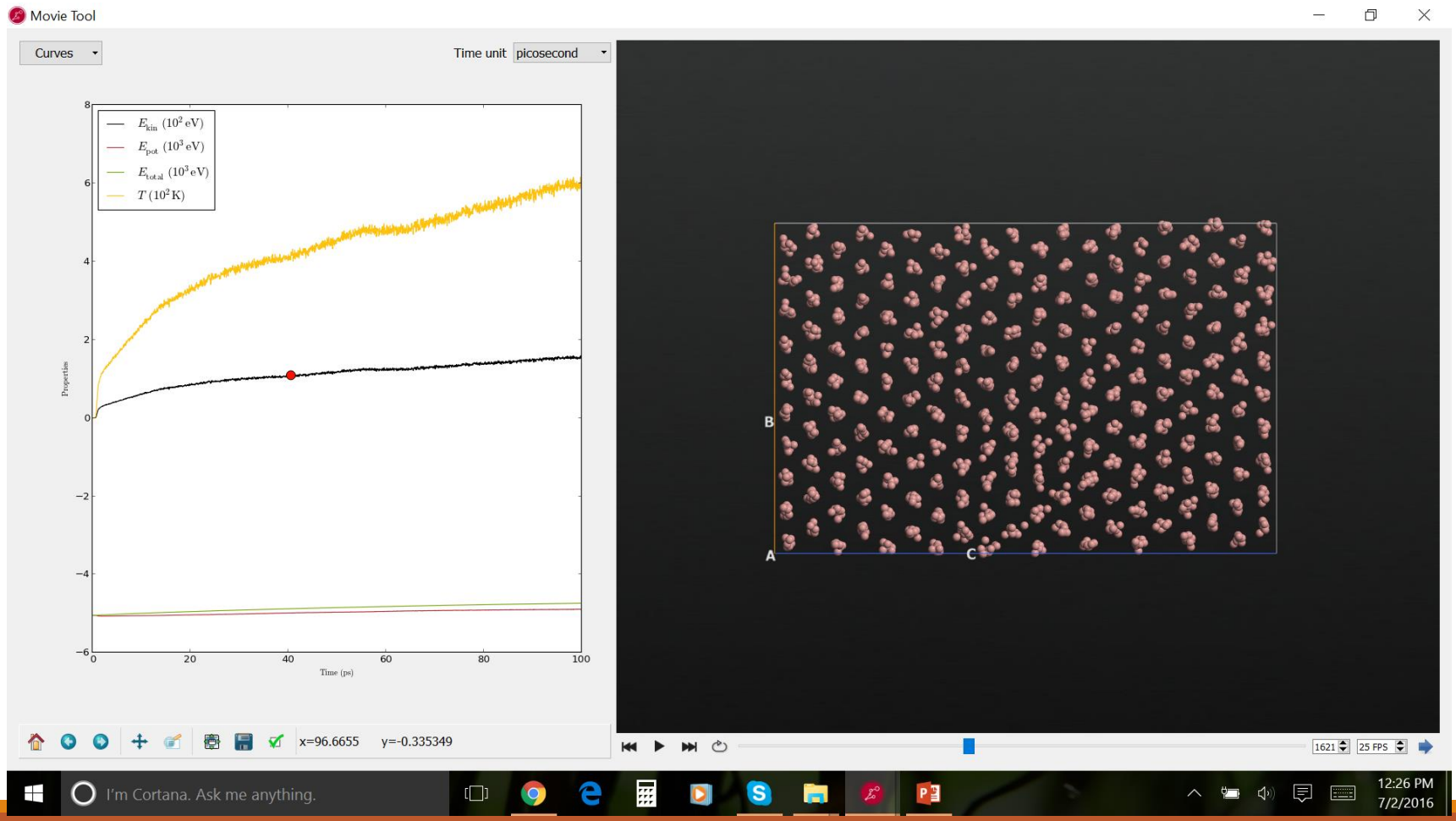
- Temperature coupling – 30000 fs
- Pressure coupling – 25 fs
- Reservoir Temp – 800 K
- Configuration velocities type initial velocity was selected
- Simulation steps – 100,000
- Indicated Melting point – 465 K



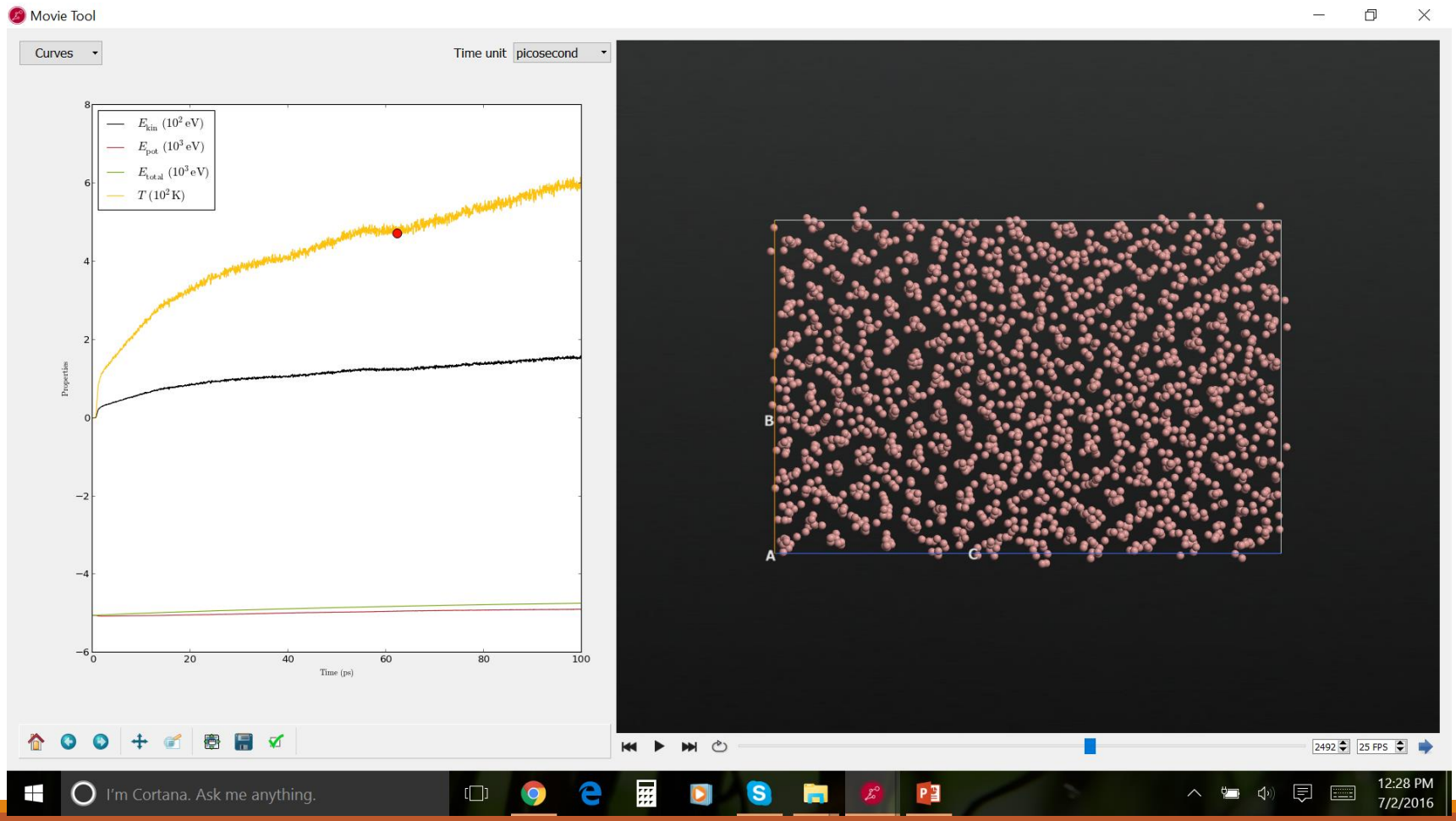
10x10x10 Indium – 20ps



10x10x10 Indium – 40ps



10x10x10 Indium – melting pt



Indium-Silicon interface

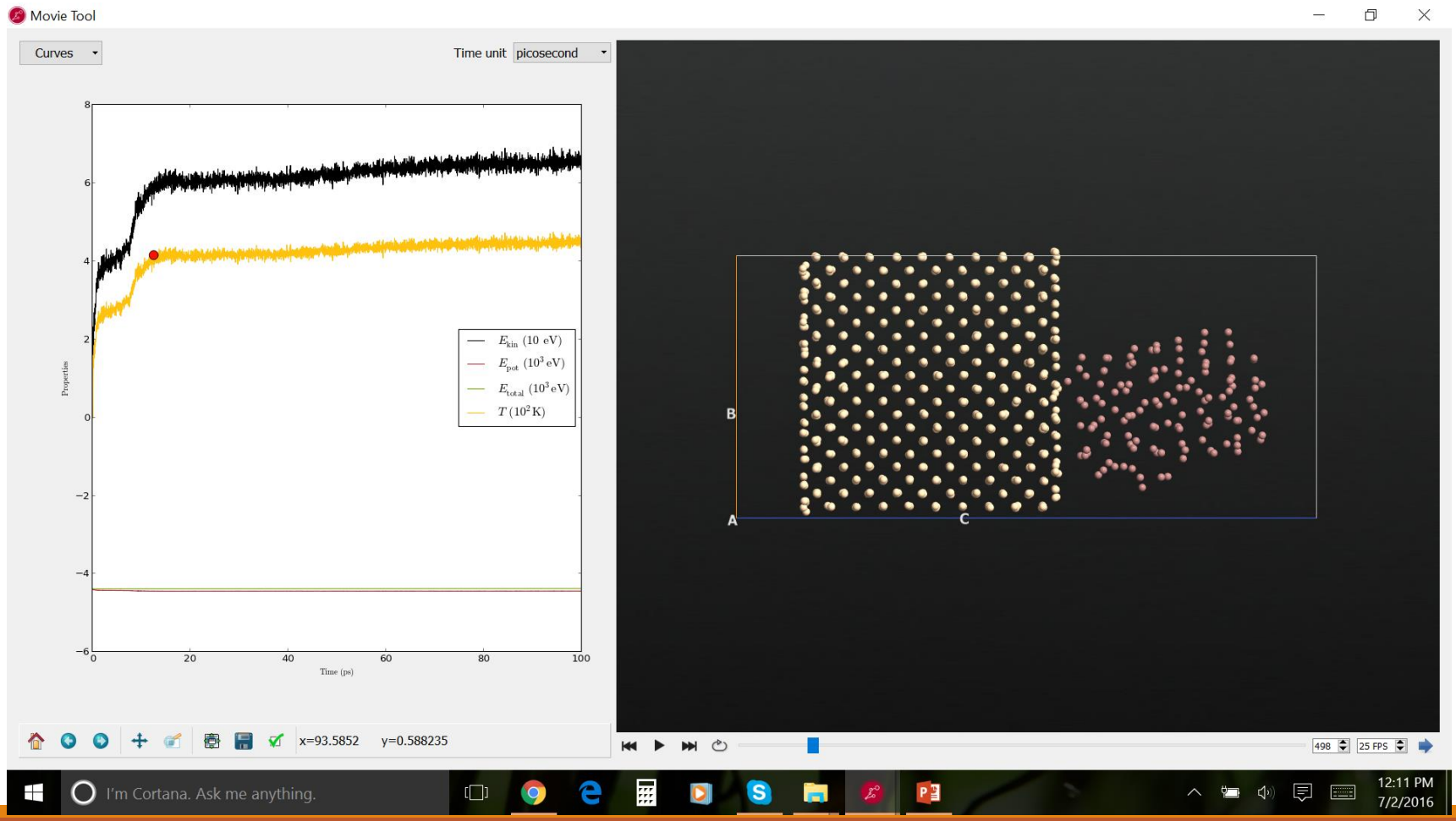
- Trying to simulate the contact characteristics of Indium on Silicon over the same 0-800 K temperature range.
- Interfacial interaction between In-Si was based on LJ potential as defined in the following paper:

http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=5767199&tag=1

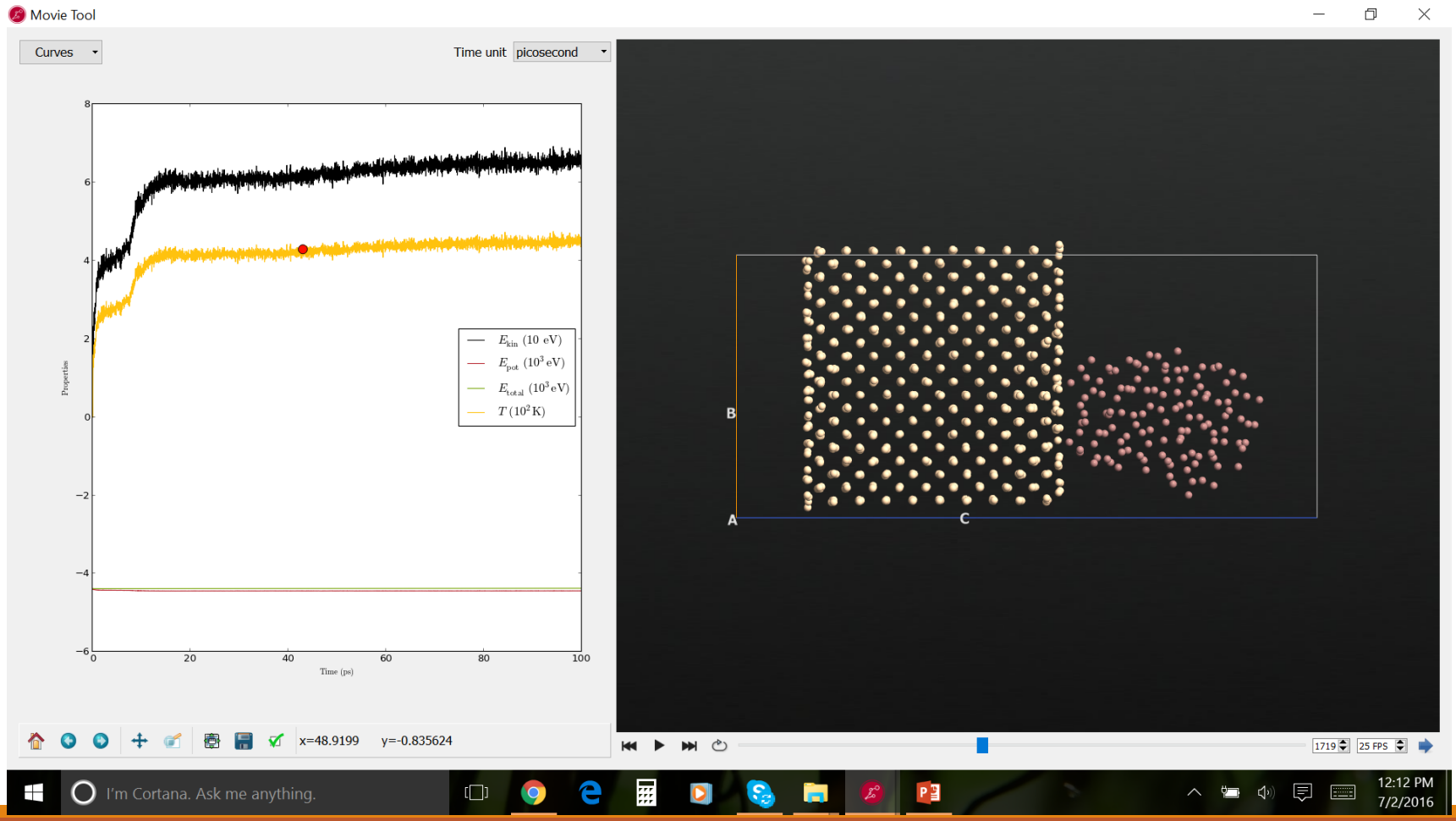
- Trying to incorporate the parameters defined in the paper into the python script, and troubleshooting the errors.
- First few simulations indicate that Indium is dewetting on Silicon surface but trying to fix the strange behavior of the Silicon atoms during the heating up process.
- Python script of the simulation shown next is attached

Indium + Silicon (alpha)_8.py

Indium-Silicon interface



Indium-Silicon interface



Indium-Silicon interface