In-Si surface Wetting – Molecular Dynamics Simulation

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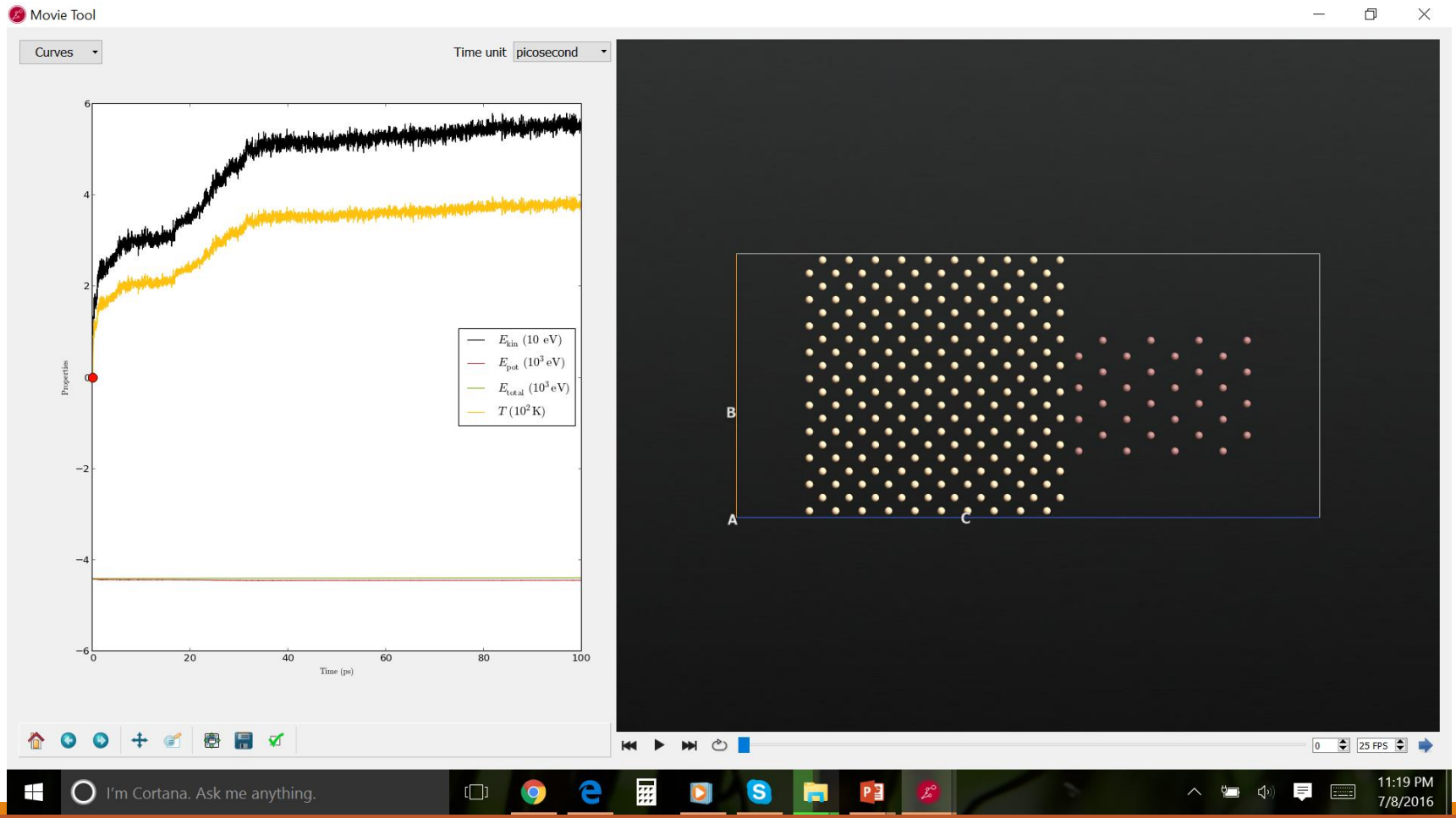
TODAY'S DATE – 08/08/2016

Indium-Silicon interface

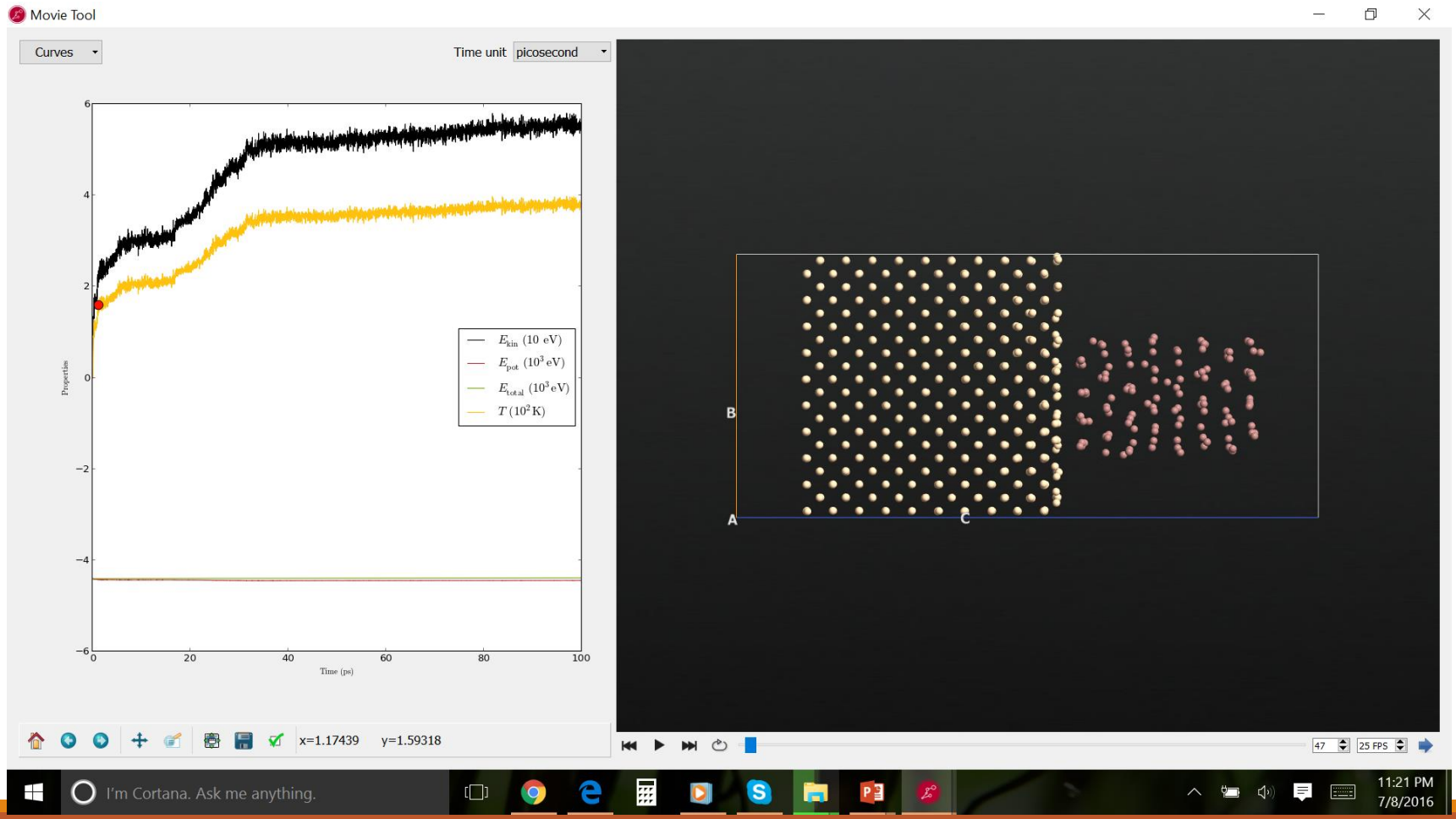
- Continued studying wetting phenomenon at Si-In interface with QuantumWise
- Based on information from literature, for the same interface the phenomenon changes from dewetting to wetting when the 'epsilon' factor of the LJ potential increases (with all other factors and operating parameters remaining the same)
- Verified this by varying the epsilon factor from 0.00865 to 0.0565 (7 simulations carried out) and the results of two of them are presented in the following slides.
- Operating Parameters used for the simulation:
  - Temperature coupling - 30,000 fs
  - Pressure coupling - 25 fs
  - No. of simulation steps - 100,000
  - Reservoir temperature - 800 K
  - NPV Bendersen MD type simulation
  - Composite compressibility - 0.0172 Gpa^{-1}

Epsilon - 0.008625 (0 ps)

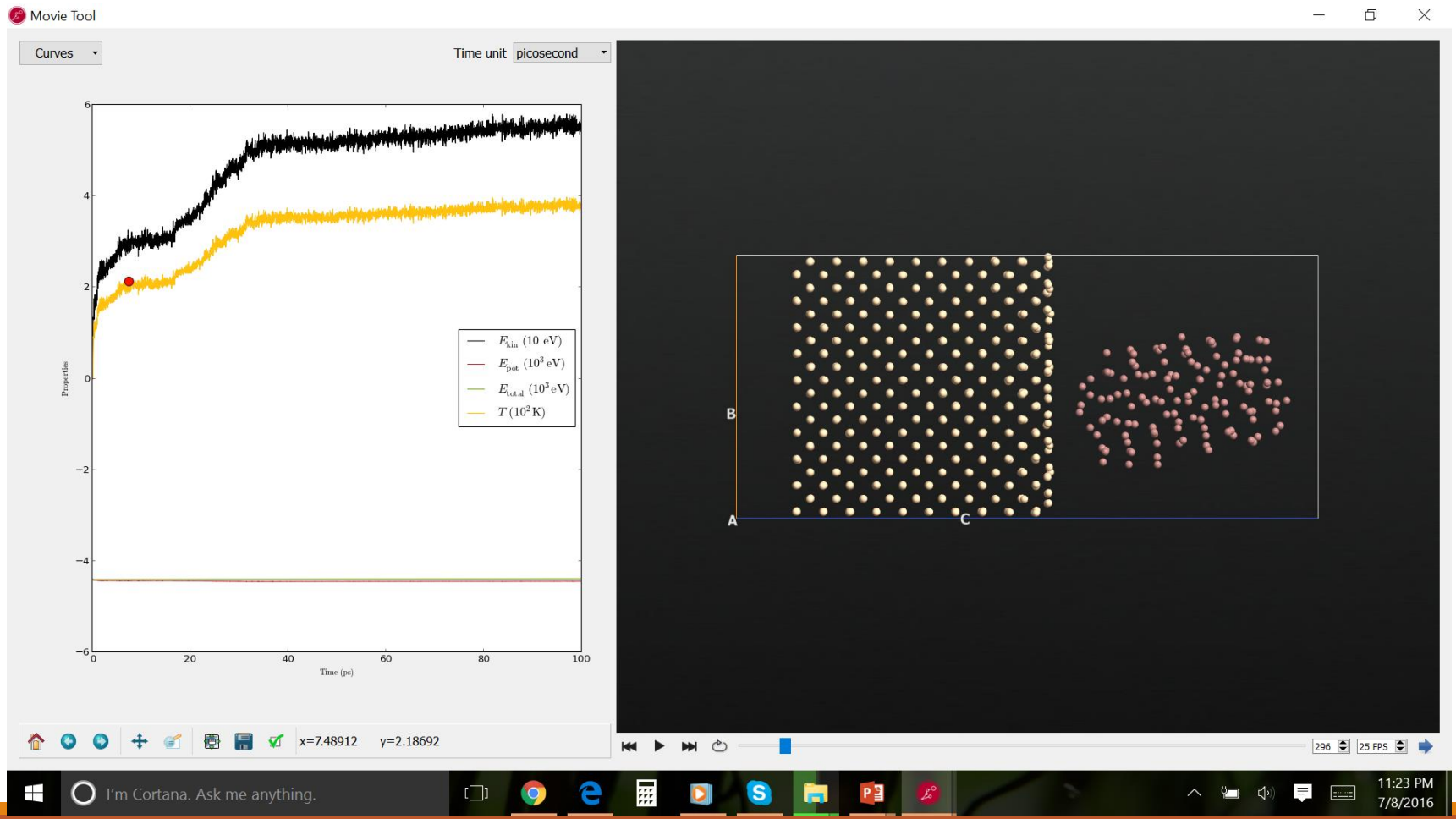
Indium + Silicon (alpha)_15.py



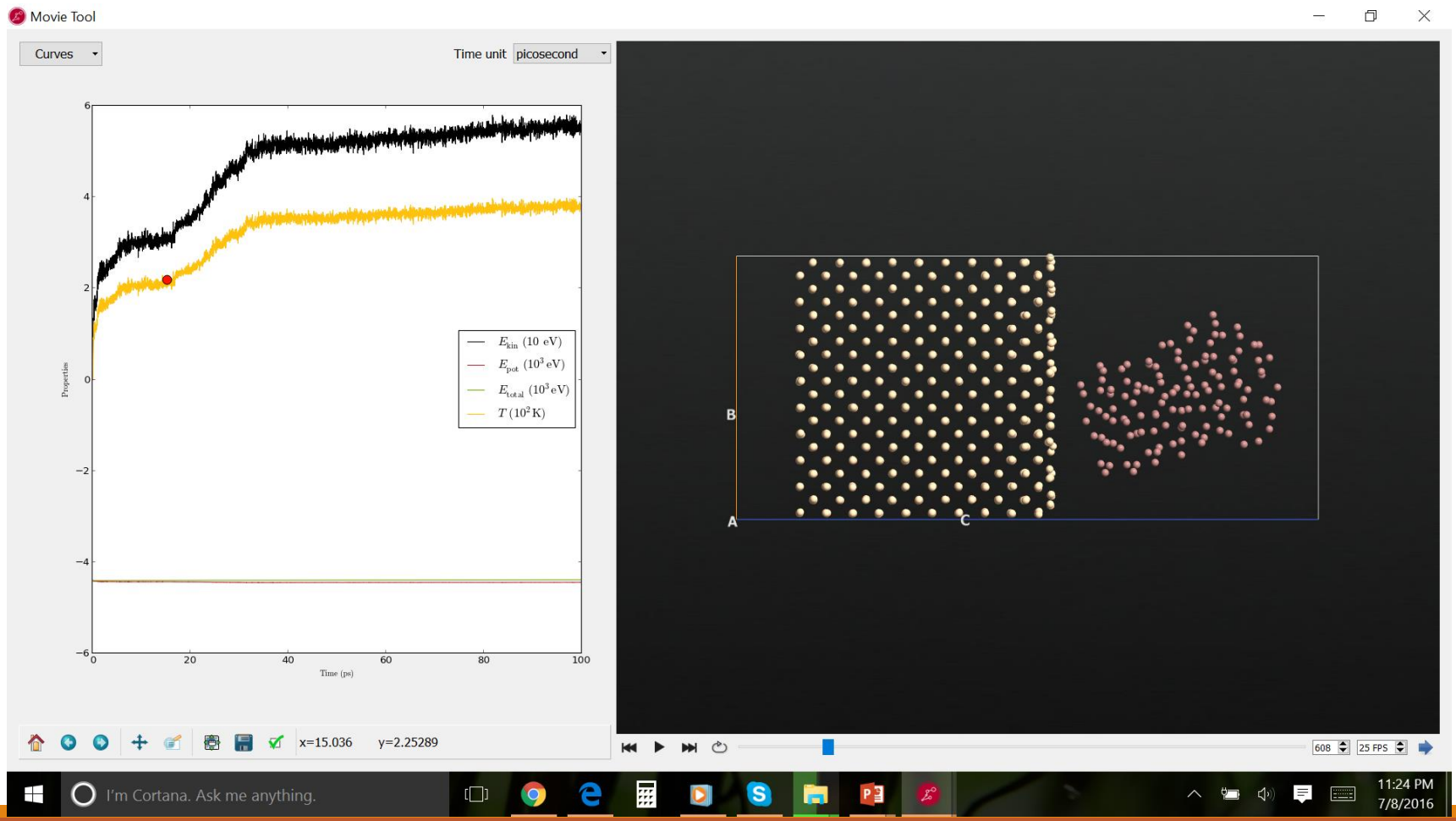
Epsilon - 0.008625 (1.17 ps)



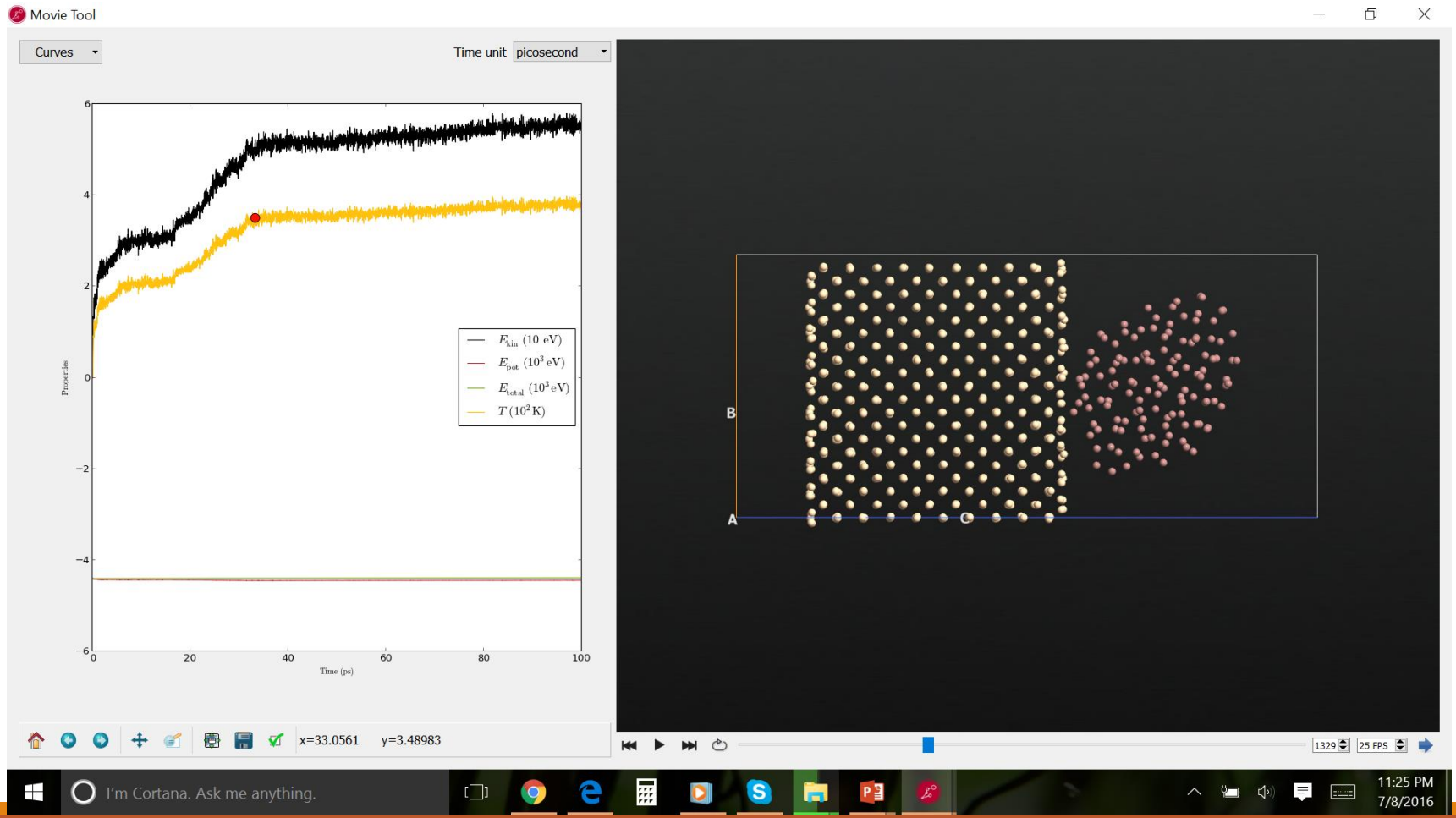
Epsilon - 0.008625 (7.5 ps)



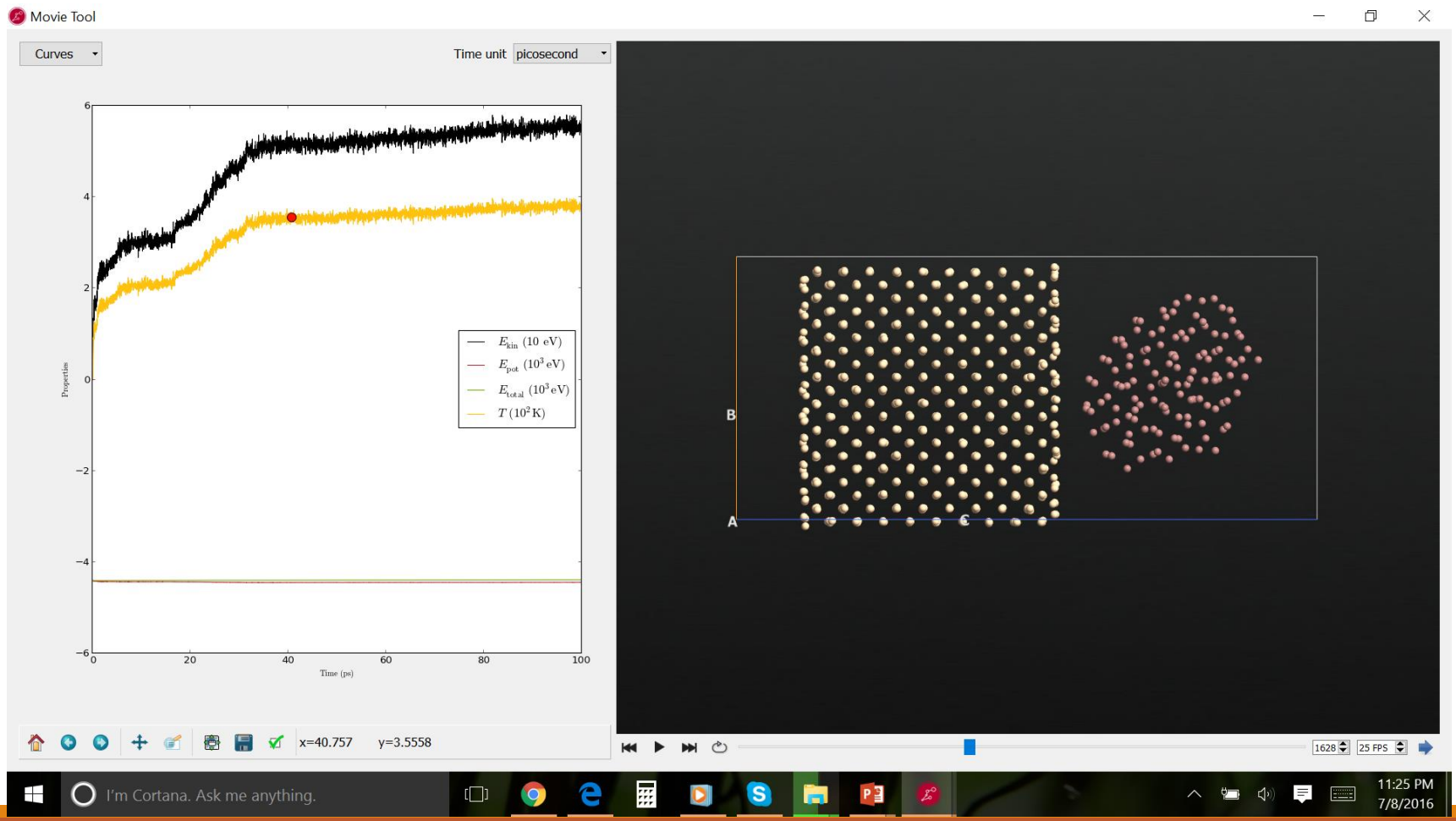
Epsilon - 0.008625 (15 ps)



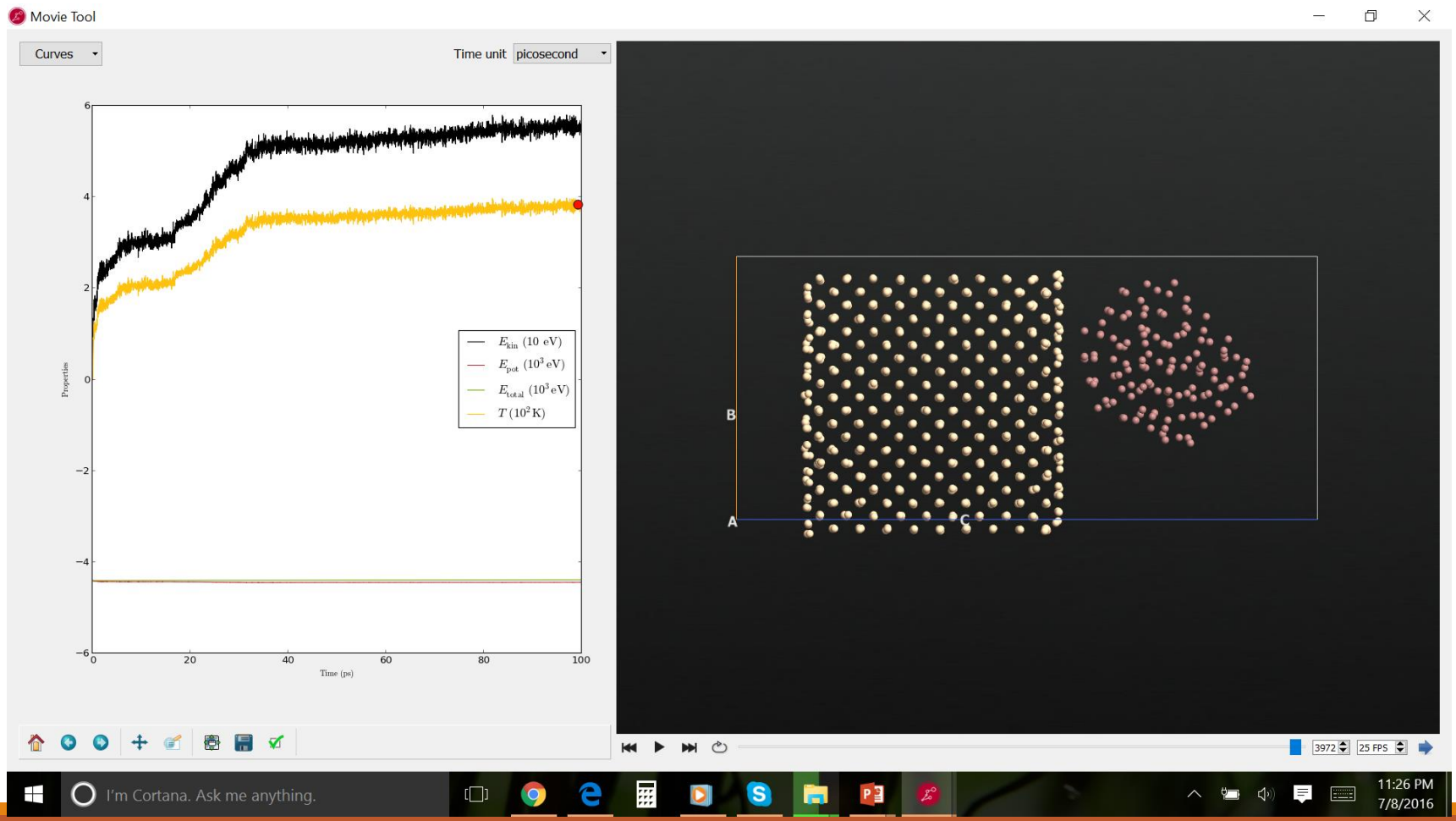
Epsilon - 0.008625 (33 ps)



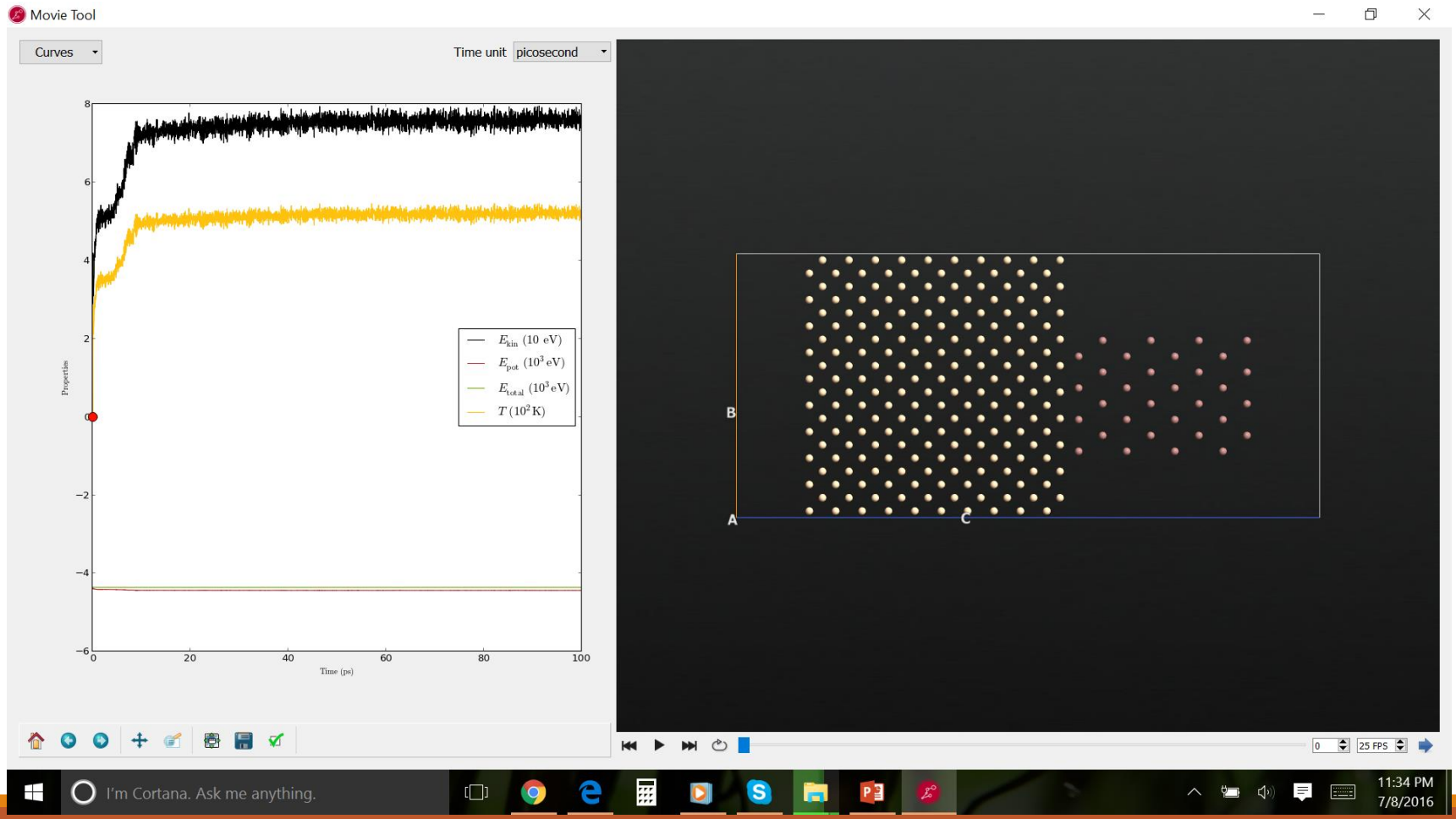
Epsilon - 0.008625 (40 ps)



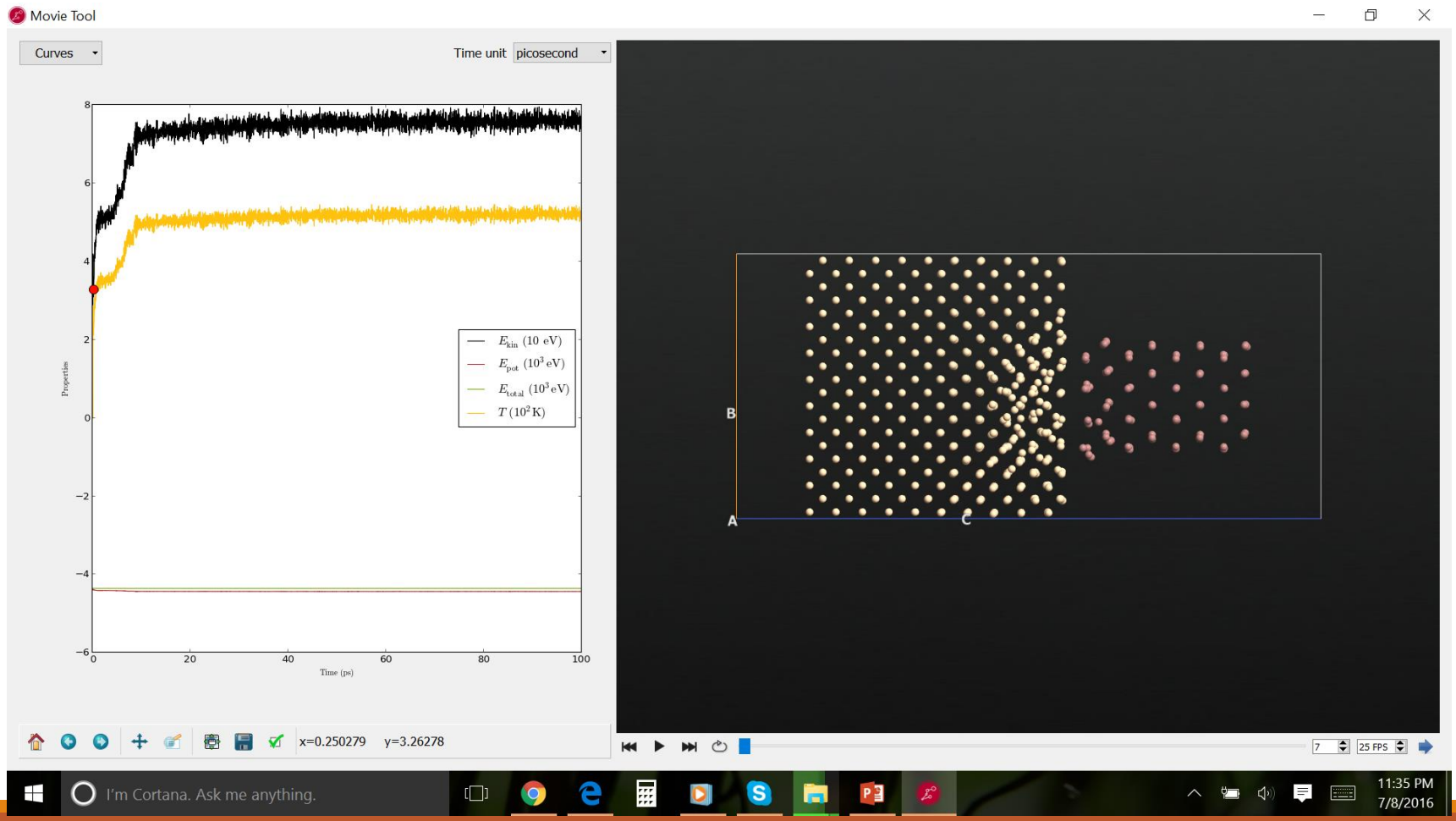
Epsilon - 0.008625 (100 ps)



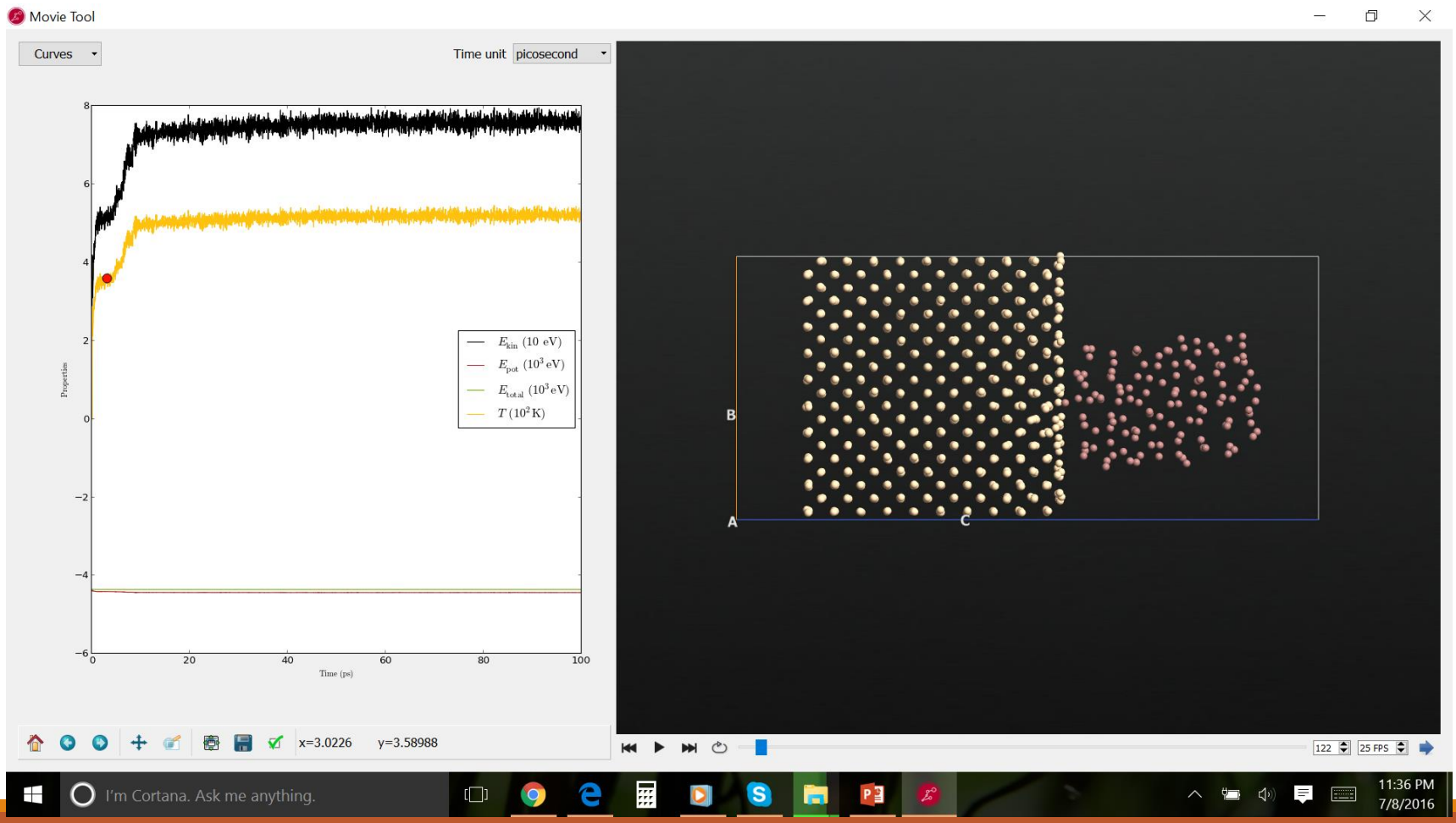
Epsilon - 0.05625 (0 ps)



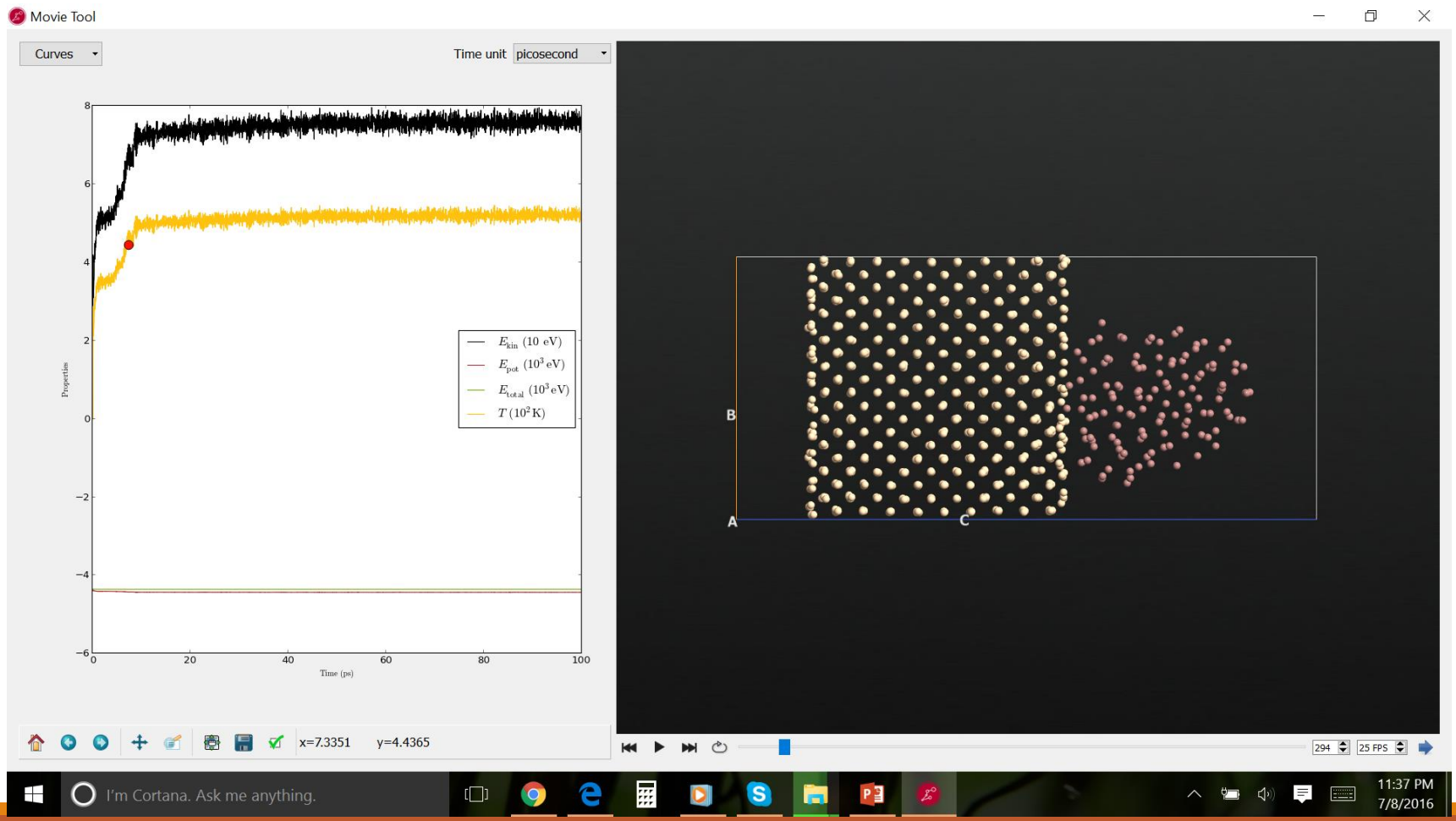
Epsilon - 0.05625 (0.25 ps)



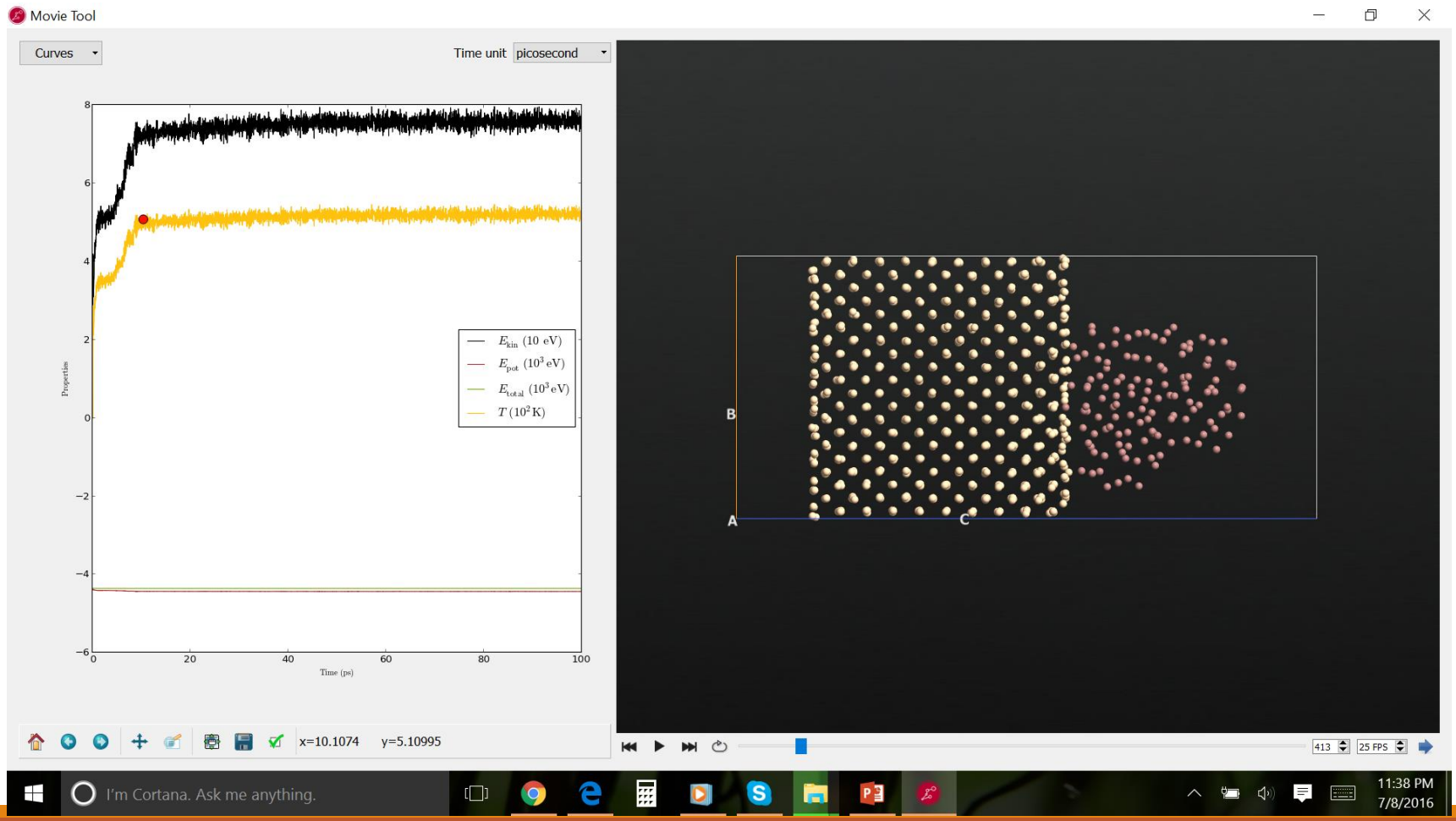
Epsilon - 0.05625 (3 ps)



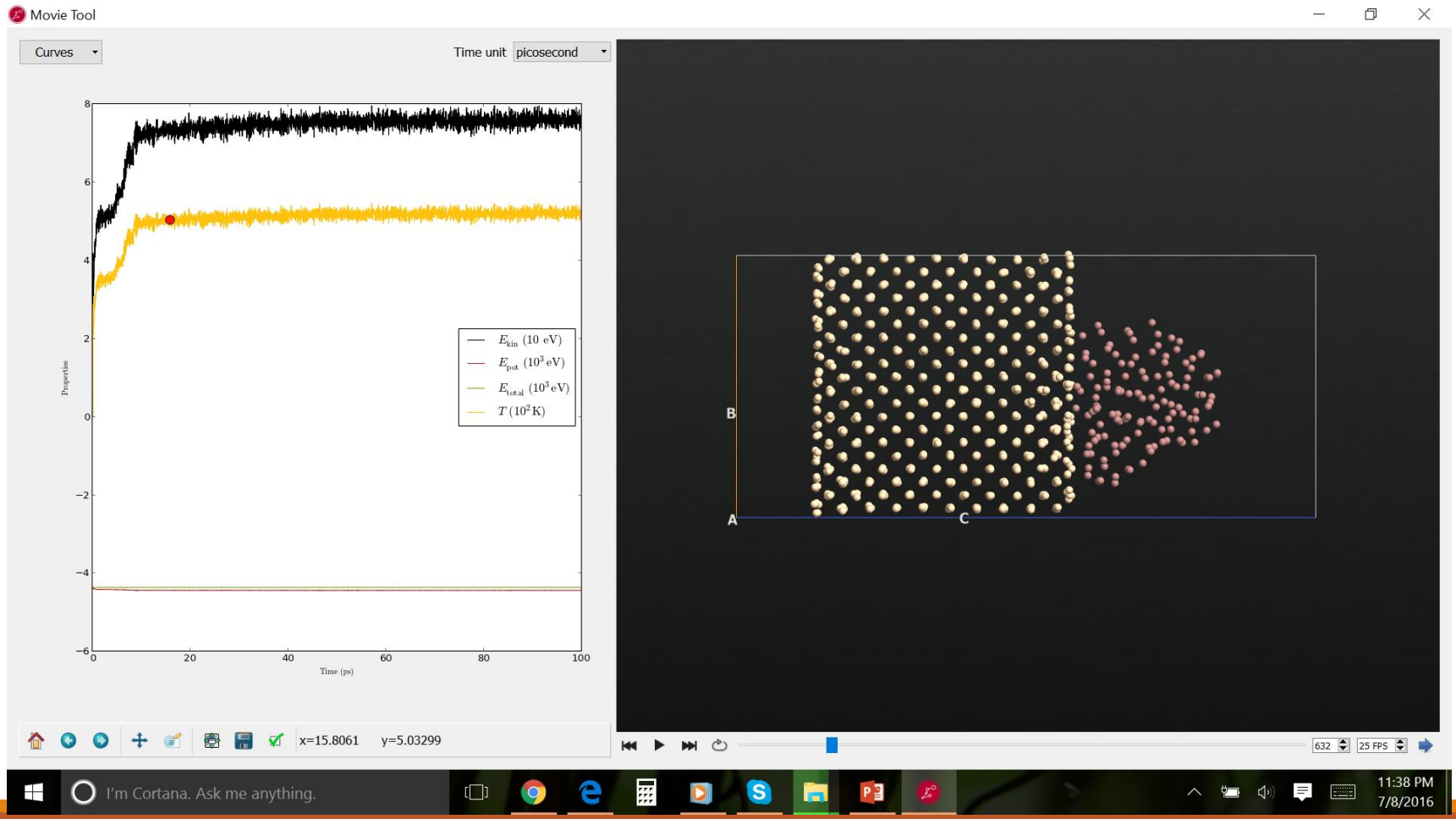
Epsilon - 0.05625 (7.3 ps)



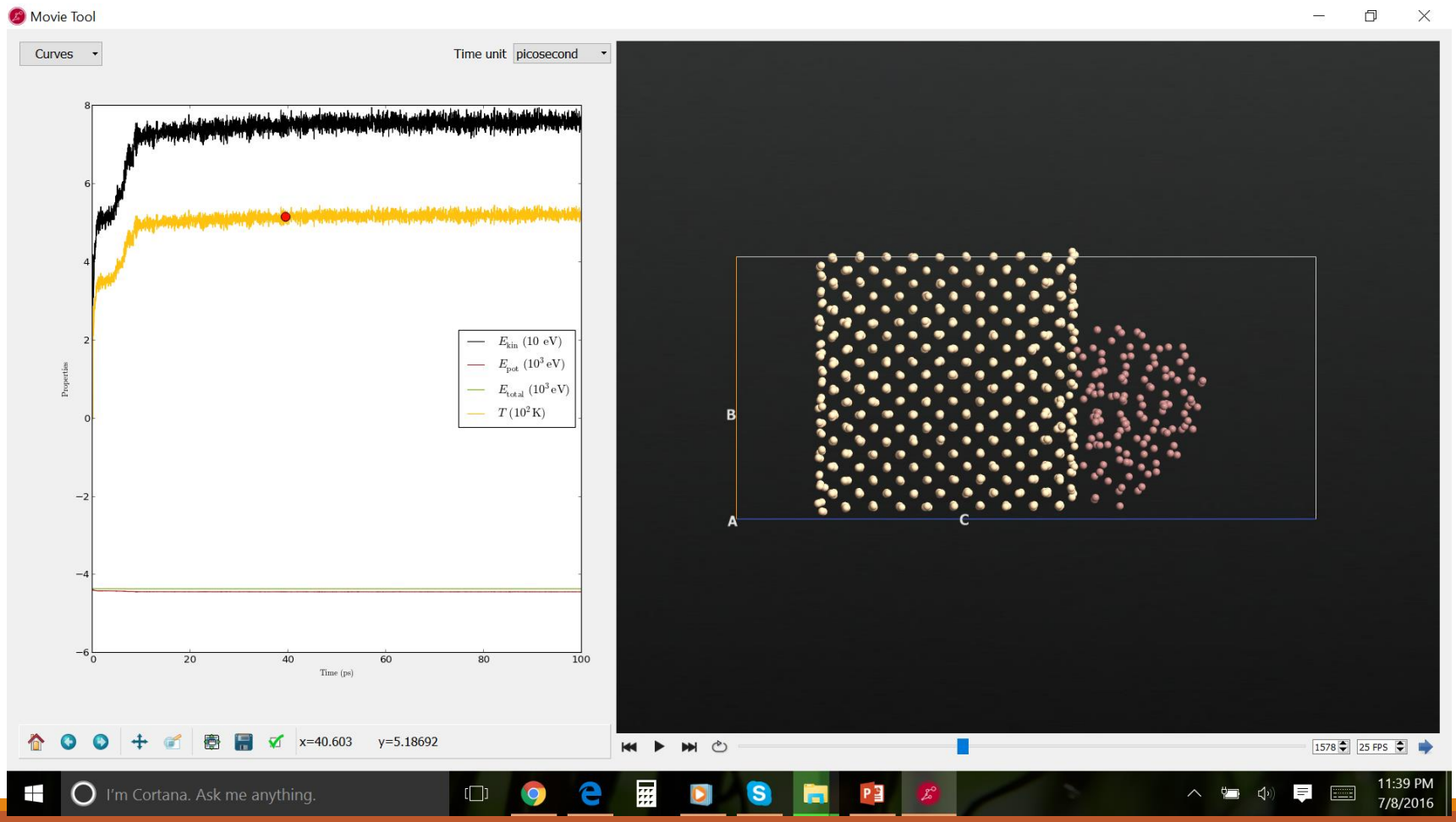
Epsilon - 0.05625 (10 ps)



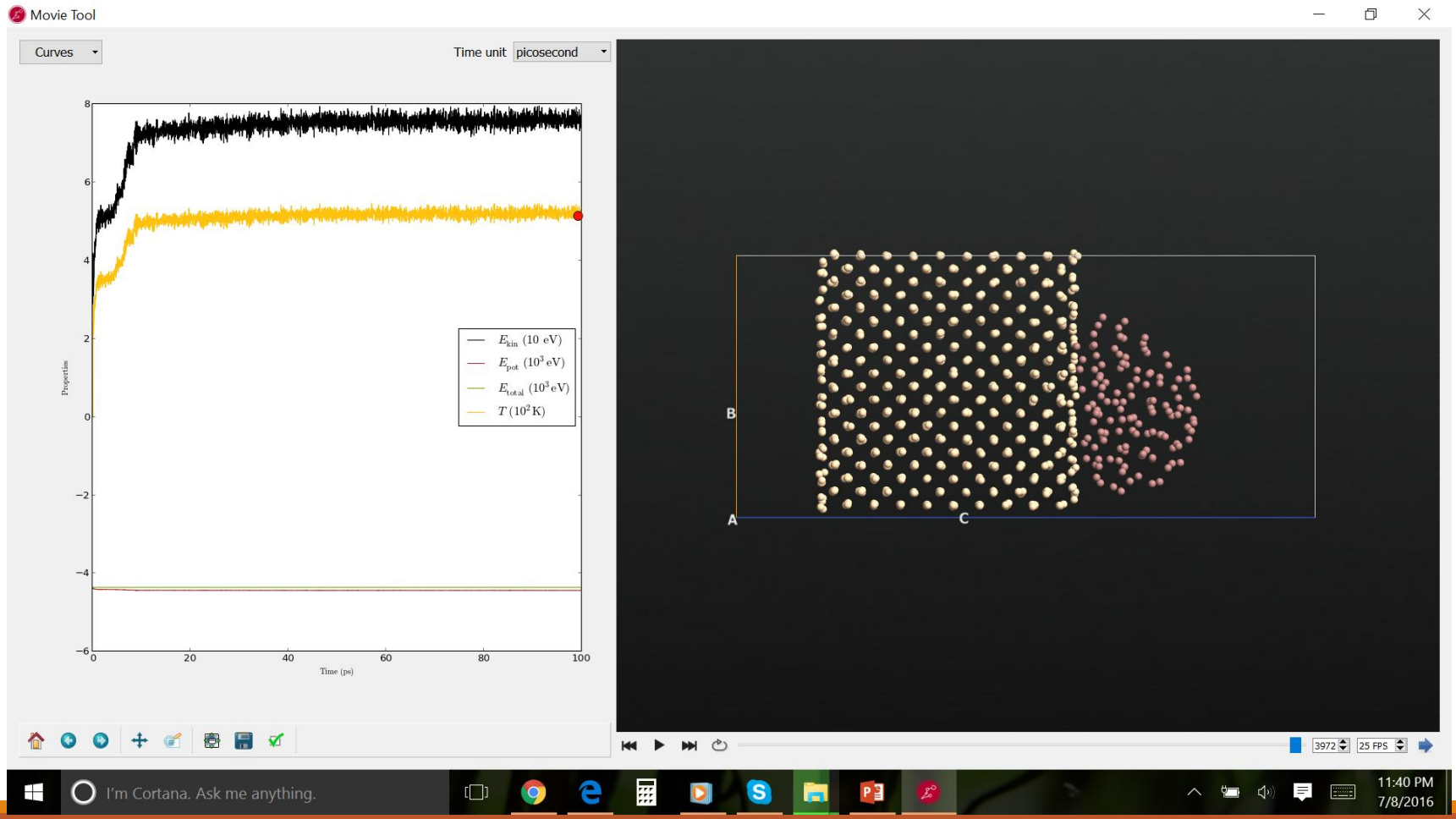
Epsilon - 0.05625 (15 ps)



Epsilon - 0.05625 (40 ps)



Epsilon - 0.05625 (100 ps)



Conclusion & path forward

- As epsilon factor was increased, the interface interaction changed from dewetting to wetting – in line with expectation
- Next effort will be simulating Moly oxide – Indium interface interaction.
- There is no published literature with defined LJ potential for MoOx-In junction.
- Plan is to come up with the parameters using DFT and pseudopotentials and we now know that epsilon is the key factor to be focused at.

Observation

- In spite of providing 100,000 steps, the composite temperature never reached the set point of 800 K in all the simulations.
- The steady state temperature achieved during each of simulations was found to increase with increase in epsilon value
- During the last week's simulation where all the LJ potential parameters were taken from published literature (epsilon = 0.0265), the steady state temperature achieved was around the melting point of Indium (~440K)
- Trying to understand the reason for this.