

Limitations of Molecular Mechanics

- Less accurate potential energy
- Cannot model bond formation or breaking
- Popular fixed-charge force fields do not account for polarization

What is Molecular Dynamics?

- Add energy to a system modeled by molecular mechanics and simulate its progress with time
- See 0:45 to 2:20 of “An Introduction to Molecular Dynamics” (<https://www.youtube.com/watch?v=ILFEqKI3sm4>)
- See a separation of alkane and water: <https://www.youtube.com/watch?v=xcMSHy3CqXA>