

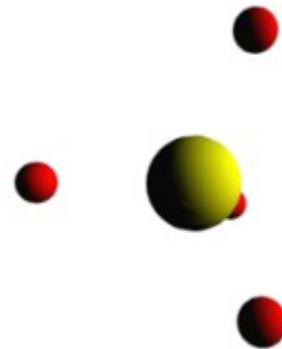
Modelling of interatomic interactions

Alexey Sokolov,
Advanced Problems in Mechanics 2012,
St. Petersburg, Russia.

Introduction

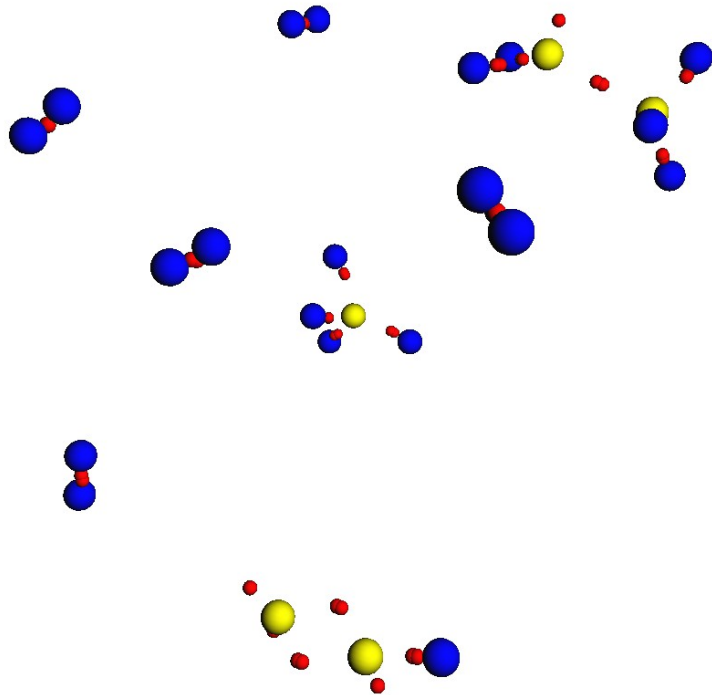
Atom representation:

- We represent atom as a number of material points one of them representing center of mass of nucleus, others representing centers of mass of electron clouds
- Electron clouds of one atom repells;
- Nucleus of different atoms repells;
- Electron clouds of different atoms attracts
bond between them is saturated



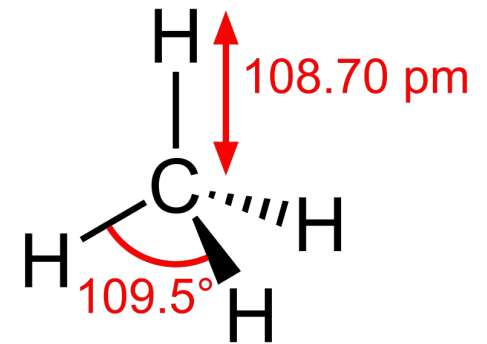
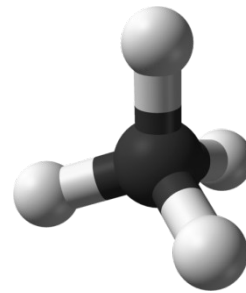
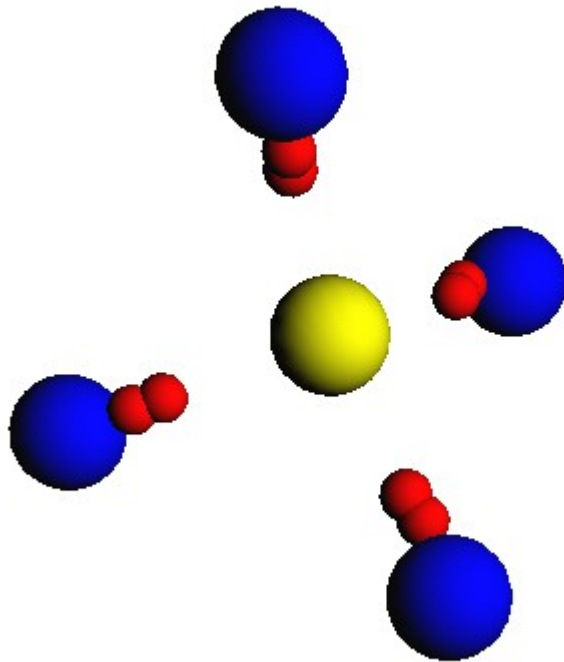
example of carbon atom

Results



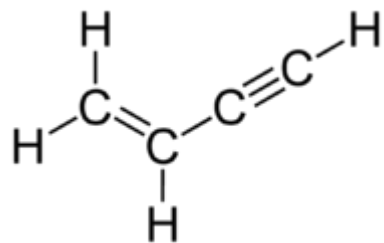
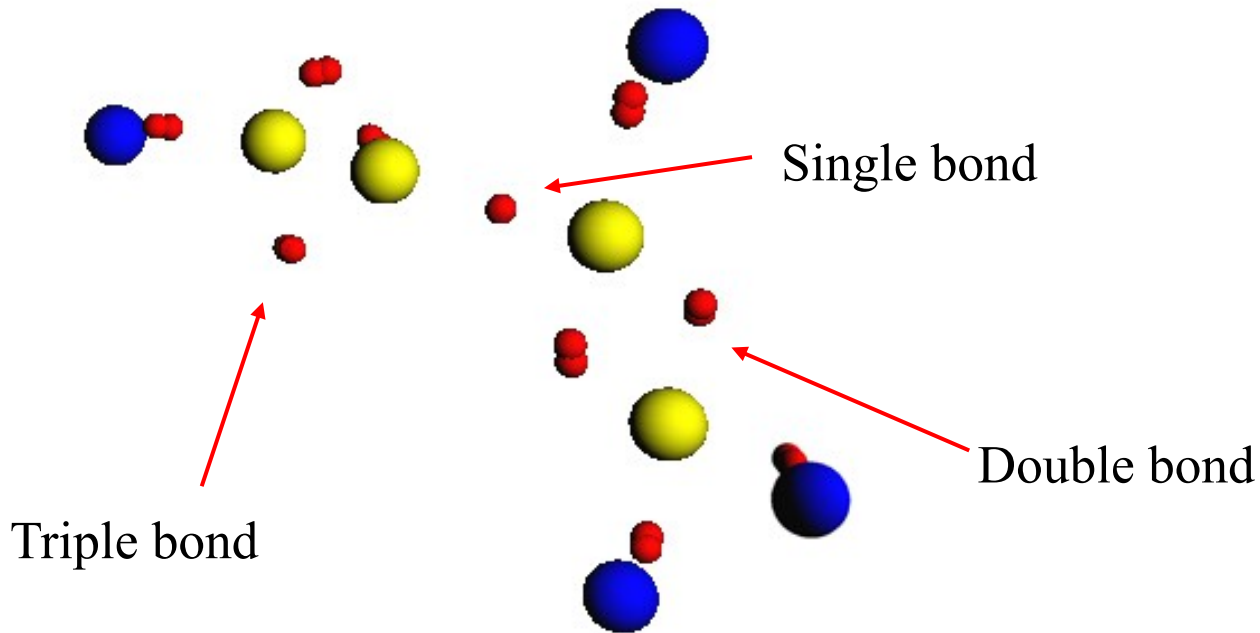
Disordered atoms
Interacted with
presented potential
self organised into
knowns chemical

Results

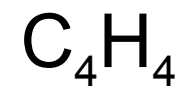


**Example of CH₄ obtained
in simulation: comparison
with classical chemical theory**

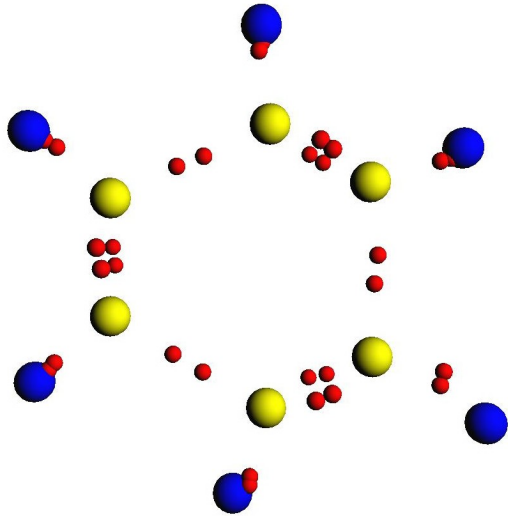
Results



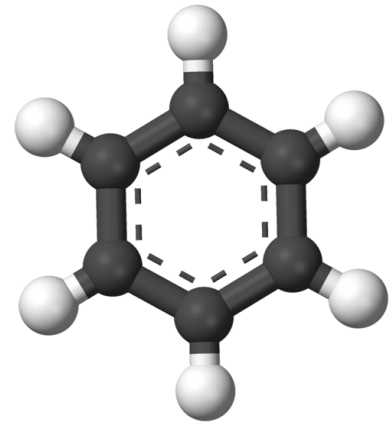
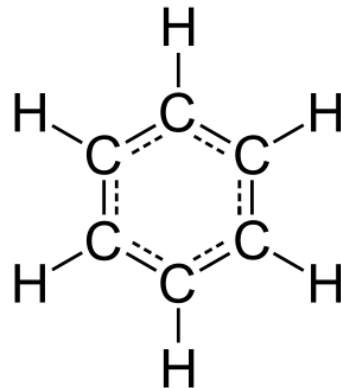
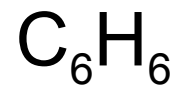
vinylacetylene



Results



- Benzol molecule



Thank you for your attention