

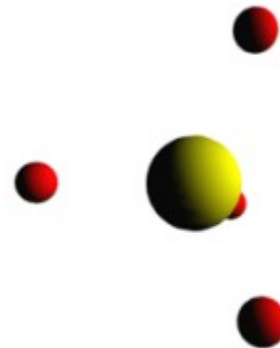
Computer modelling of interatomic interactions

Alexey Sokolov,
Advanced Problems in Mechanics 2013,
St. Petersburg, Russia.

Introduction

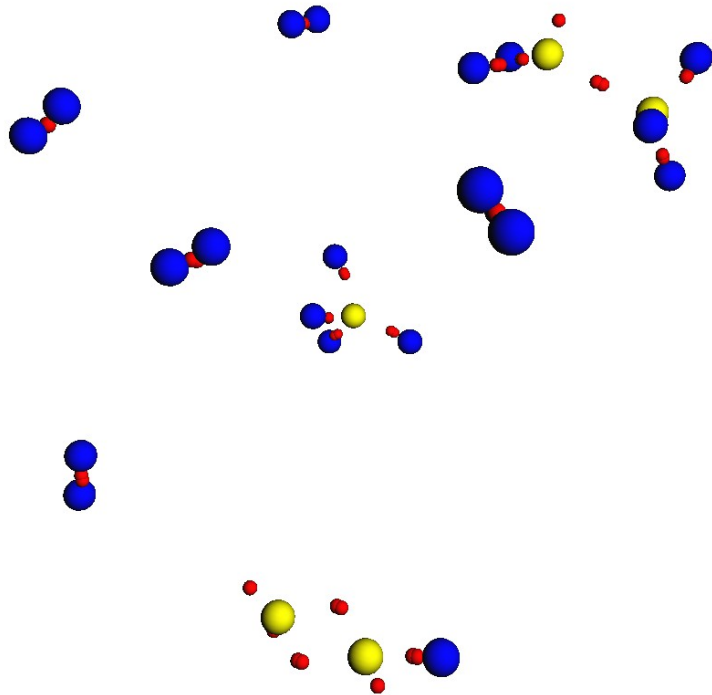
Atom representation:

- 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 repels;
- Nucleus of different atoms repels;
- Electron clouds of different atoms attracts
bond between them is saturated



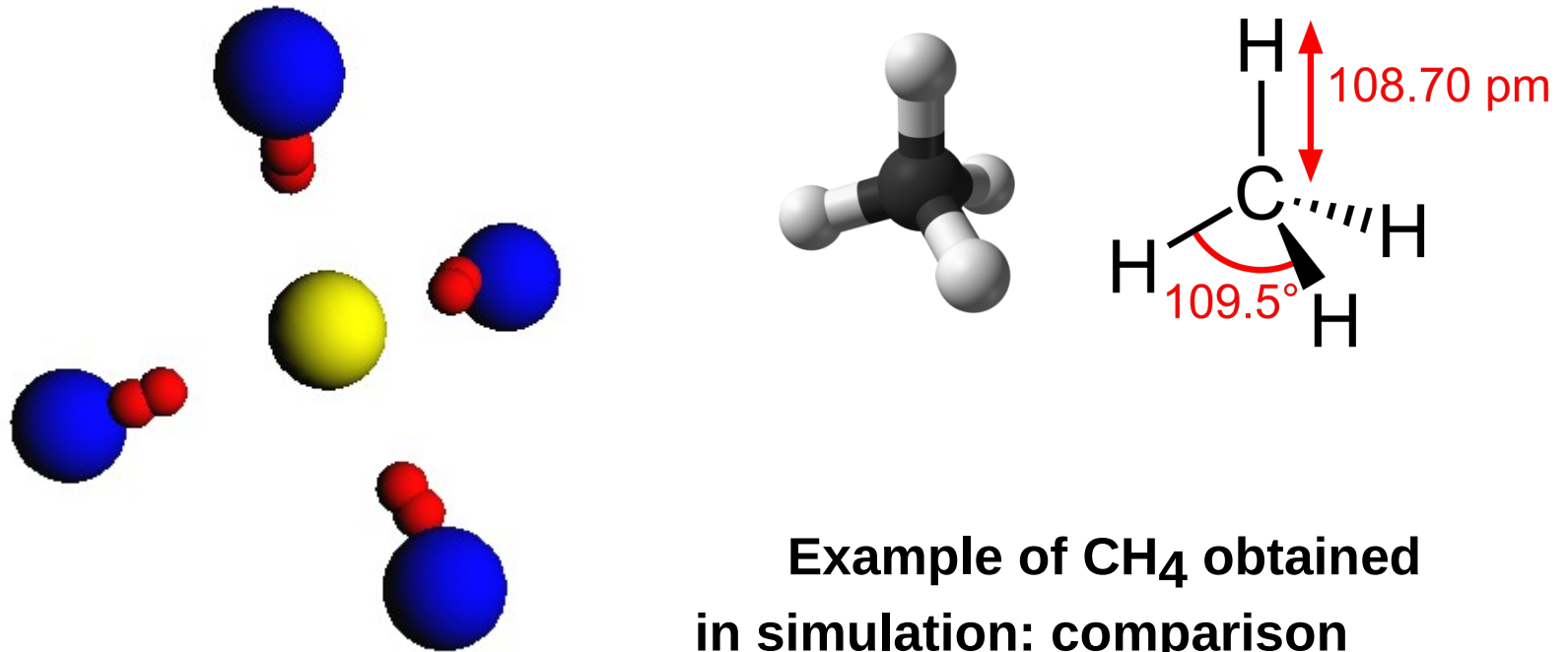
example of carbon atom

Results



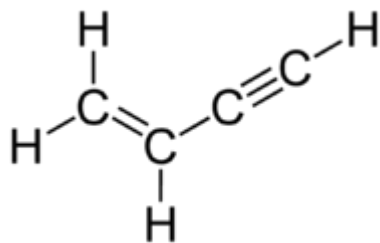
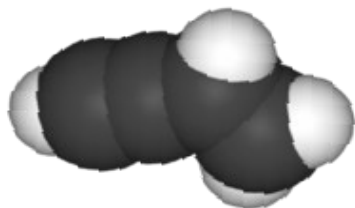
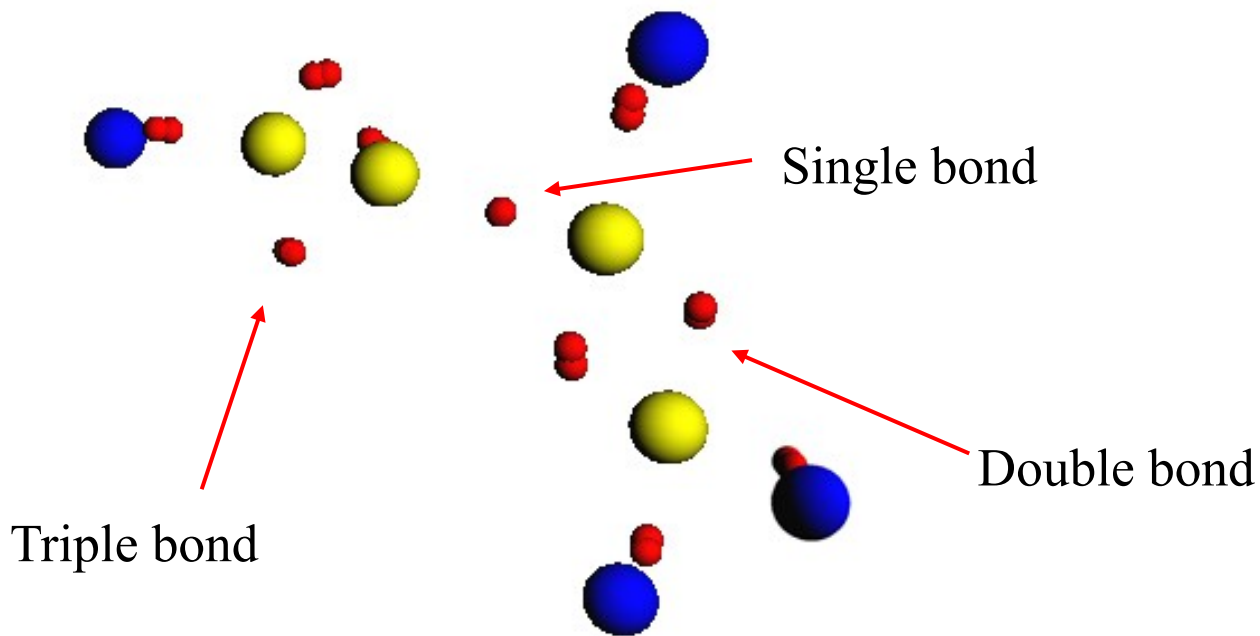
Disordered atoms
Interacted with
presented potential
self organised into
known chemical

Results

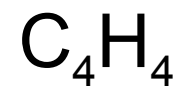


**Example of CH_4 obtained
in simulation: comparison
with classical chemical theory**

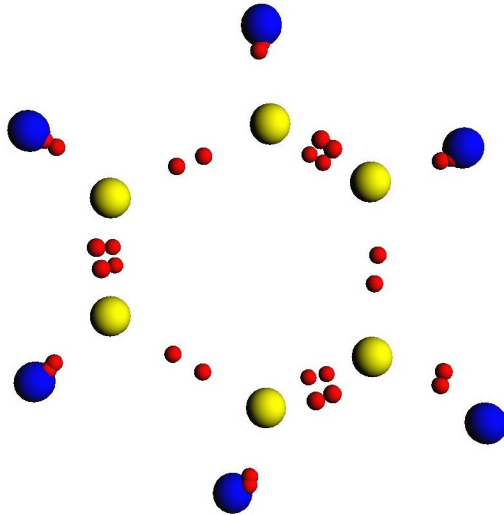
Results



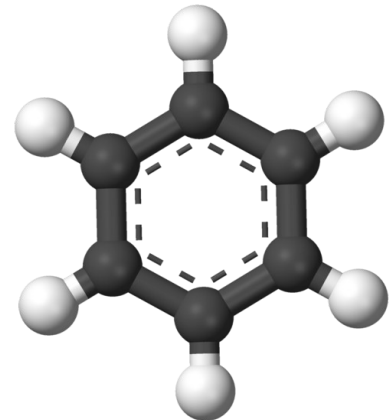
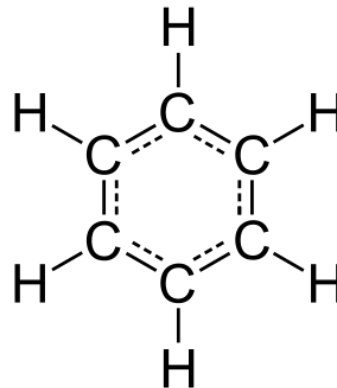
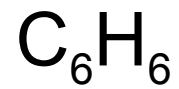
vinylacetylene



Results



- Benzol molecule



Thank you for your attention