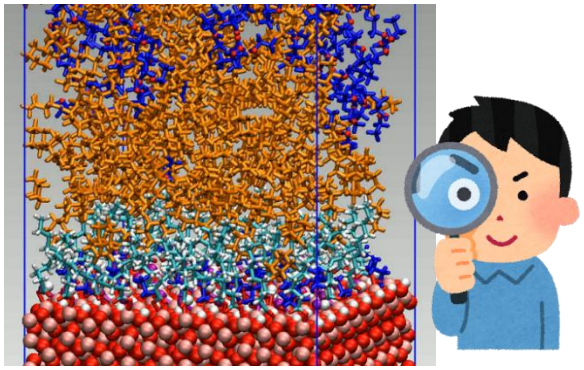
Visualizing the nanoscale phenomena with molecular dynamics simulation

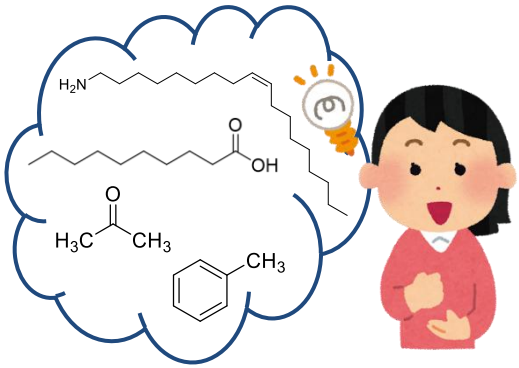
Outline

In the design of highly-functional materials such as nanofluids and polymer nanocomposites, it is important to understand the nanoscale phenomena and the affinity between substances. Let's visualize dynamics and states of molecules at nanoscale interfaces using **molecular dynamics simulations**. By performing simulations based on the laws of nature, students can learn how to design novel materials through evaluating the affinity between substances and clarifying the relationship between molecular structure and material properties.

Computer simulation



Evaluation of
interfacial structure and affinity



Ideas for novel design of materials

PC beginners are welcomed. All the staff will support you.
An interest in chemistry is recommended.

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