

General Features in Avogadro

Spoken Tutorial Project

<http://spoken-tutorial.org>

National Mission on Education through ICT

<http://sakshat.ac.in>

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Learning Objectives



Learning Objectives

- ▶ Proton transfer in compounds by changing pH values



Learning Objectives

- ▶ **Proton transfer in compounds by changing pH values**
- ▶ **Load crystal structures**



Learning Objectives

- ▶ Proton transfer in compounds by changing pH values
- ▶ Load crystal structures
- ▶ Show various Miller planes



Learning Objectives

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- ▶ Build super cells



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System Requirement



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- ## ► Ubuntu Linux OS v 14.04



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- ▶ **Ubuntu Linux OS v 14.04**
- ▶ **Avogadro version 1.1.1**



Pre-requisites



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► Avogadro interface



Pre-requisites

- ▶ **Avogadro** interface
- ▶ For relevant tutorials, visit our website
www.spoken-tutorial.org
- ▶ Example files used in this tutorial are provided as code files



Miller Indices



Miller Indices



Miller Indices

- ▶ Miller indices are a set of three numbers(hkl)



Miller Indices

- ▶ Miller indices are a set of three numbers(hkl)
- ▶ Used to specify directions and internal planes in crystal systems



Nanotubes



Nanotubes

- ▶ A nanotube is a nanometer-scale tube-like structure



Nanotubes

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- ▶ Examples of different types of nanotubes are:



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 - ▶ Boron carbon nitrogen



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 - ▶ Carbon



Nanotubes



Nanotubes

A carbon nanotube

- ▶ is a miniature cylindrical carbon structure



Nanotubes

A carbon nanotube

- ▶ is a miniature cylindrical carbon structure
- ▶ that has hexagonal graphite molecules attached at the edges



Summary

- ▶ Proton transfer in compounds by changing pH values
- ▶ Load crystal structures from crystal library
- ▶ Show various Miller planes
- ▶ Build super cells
- ▶ Show geometries in coordination compounds
- ▶ Build nanotubes



Assignment

As an assignment

- 1. Load AgCl crystal structure and show its Miller planes**
- 2. Load structures from coordination library and show geometries**
- 3. Build a nanotube with chirality index 9,9**



About the Spoken Tutorial Project

- ▶ Watch the video available at http://spoken-tutorial.org/What_is_a_Spoken_Tutorial
- ▶ It summarises the Spoken Tutorial project




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Acknowledgements

- ▶ Spoken Tutorial Project is a part of the Talk to a Teacher project
 - ▶ It is supported by the National Mission on Education through ICT, MHRD, Government of India
 - ▶ More information on this Mission is available at <http://spoken-tutorial.org/NMEICT-Intro>
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- The logo of the Spoken Tutorial project, featuring a stylized orange and black circular design with white curved lines.

