The Concord Consortium

The Constructive Chemistry Project

A Visual Approach to Nanotechnology Education

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WHERE DISCOVERIES BEGIN
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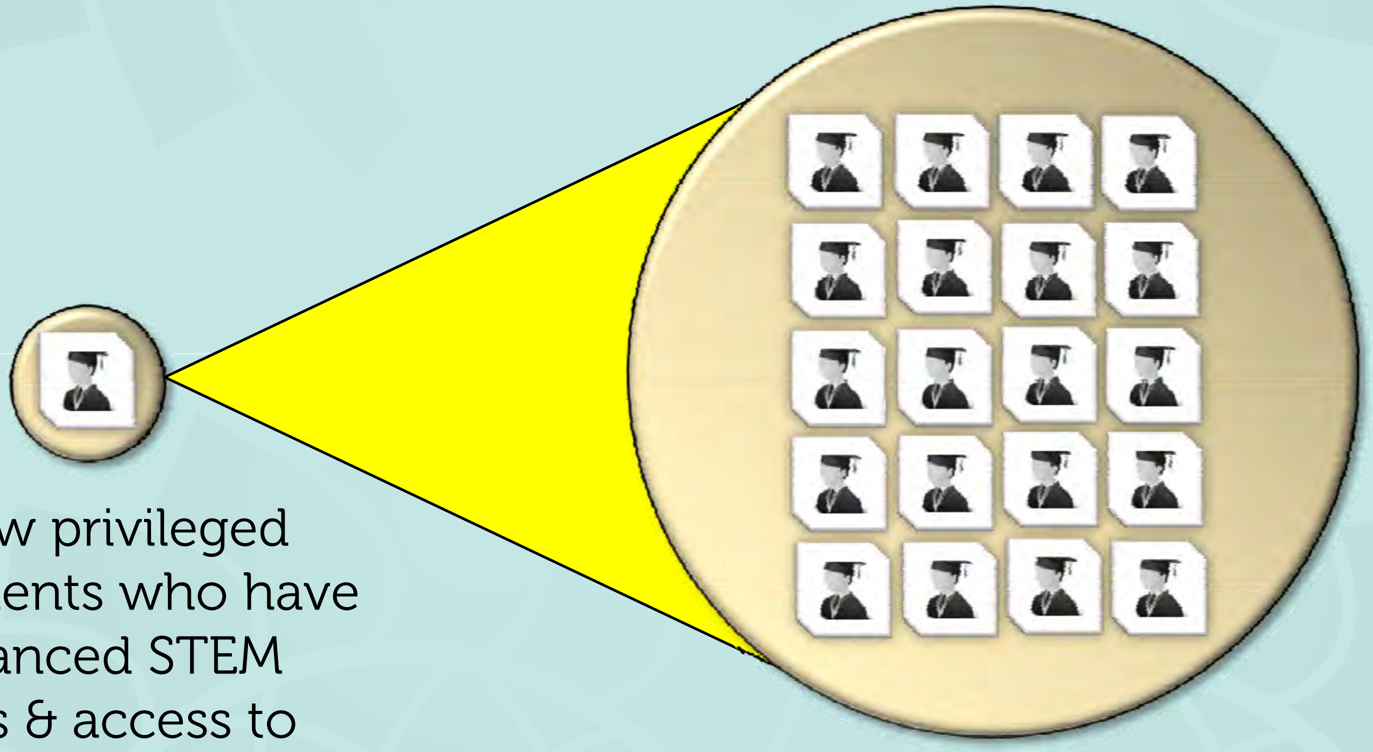
Goal

To provide a more accessible way to learn nanotechnology

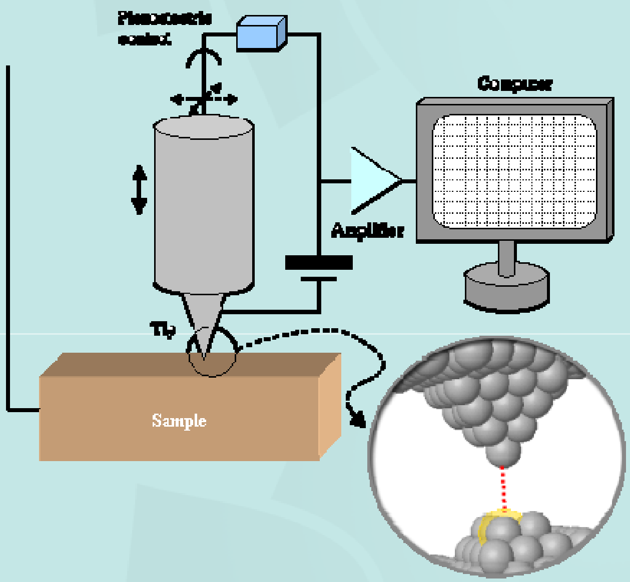


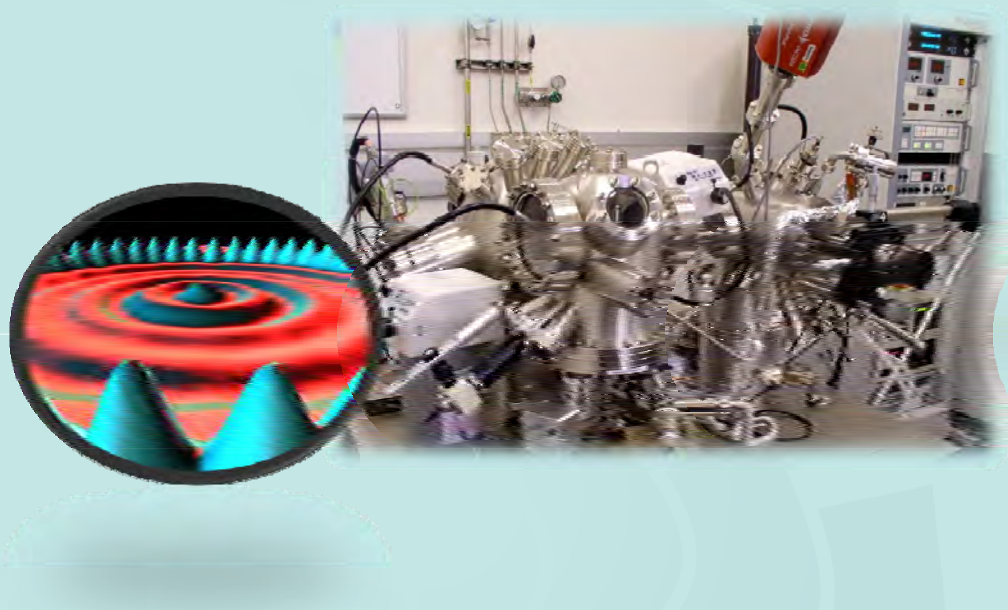
A few privileged students who have advanced STEM skills & access to research labs

"Cast a wider net":
Teach nanotechnology to many K-14 students

Problem #1

Many nanotechnology experiments are currently not possible to conduct in K-12 schools or community colleges.





Hands-on opportunities for K-14 students are scarce – Scanning tunneling microscopes and atomic force microscopes are not coming to schools any time soon.

Problem #2

Advanced mathematics used to depict and connect nanoscience concepts is not appropriate to K-12 students.

$$i\hbar \frac{\partial}{\partial t}\psi(r,t) = -\frac{\hbar^2}{2m}\nabla^2\psi(r,t) + V(r)\psi(r,t)$$

$$S = k_B \ln\Omega$$

$$m_i \ddot{R}_i = -\nabla_i V(R_1, R_2, \ldots\ldots, R_n)$$

Formal treatments commonly used in college textbooks rely on students' mathematical thinking ability to attain an integrated, deep conceptual understanding.

Learning the concept without doing the math

Nanoscience is governed by physics equations, which can be used to construct virtual labs for doing computational experiments.

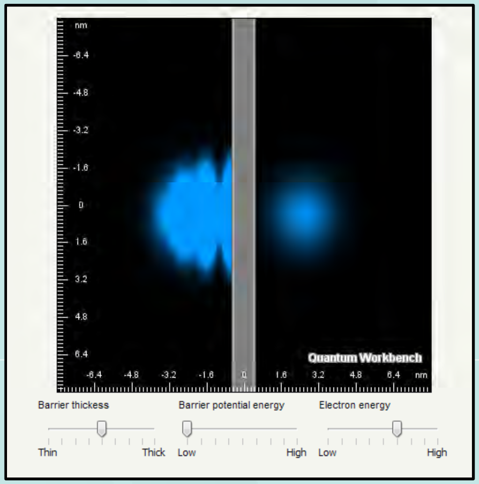
$$i\hbar \frac{\partial}{\partial t}\psi(r,t) = -\frac{\hbar^2}{2m}\nabla^2\psi(r,t) + V(r)\psi(r,t)$$

$$T = \frac{exp\left\{-2\int_{x_1}^{x_2}\sqrt{\frac{2m}{\hbar^2}\left[V(x)-E\right]}dx\right\}}{\left\{1+\frac{1}{4}exp\left[-2\int_{x_1}^{x_2}\sqrt{\frac{2m}{\hbar^2}\left[V(x)-E\right]}dx\right]\right\}^2}$$

An example

Quantum tunneling

Let the computer do the math and visualize the results with comprehensible graphics.



Learn with math

vs.

Learn with a visual simulation

Conceptual learning through mentally manipulating abstract equations (hard) can be achieved through manipulating visual simulations (easy).

Virtual labs for learning nanotechnology

What learning from conducting real experiments in real labs can be achieved by conducting computational experiments in virtual labs?

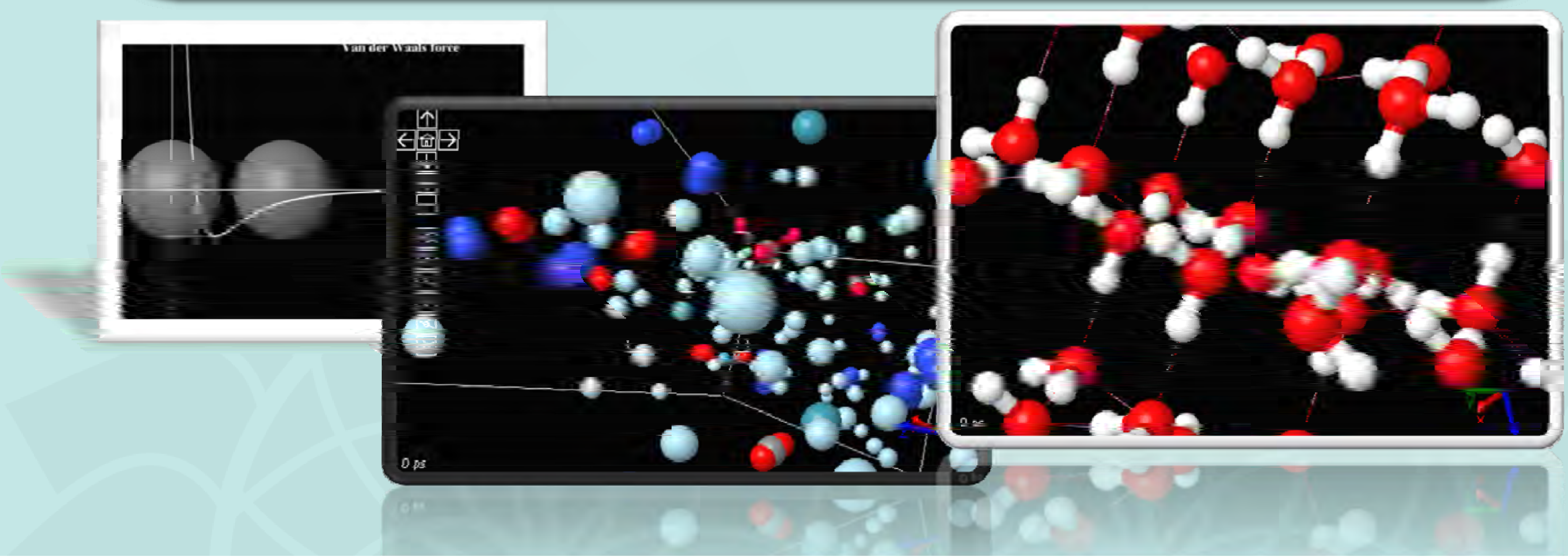
	Real labs	Virtual labs
Open-endedness	Yes	Yes
Data collection and analysis	Yes	Yes
Inquiry support	Yes	Yes
Design support	Yes	Yes
Realness	Yes	No
Hands-on skills	Yes	No

(These comparisons are based on idealized cases.)

Mathematical Models for Nano Simulations

Richard Feynman

"If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generations of creatures, what statement would contain the most information in the fewest words? I believe it is the atomic hypothesis . . . that all things are made of atoms—**little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another**. In that one sentence, you will see, there is an enormous amount of information about the world, if just a little imagination and thinking are applied."



Molecular Dynamics

Newton's Equation of Motion (classical mechanics)

$$m_i \ddot{R}_i = -\nabla_i V(R_1, R_2, \ldots\ldots, R_n)$$

Molecular mechanics: Intra- & intermolecular interaction potentials

$$V_{LJ} = \frac{1}{2}\sum_{i,j,i\neq j} 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{R_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{R_{ij}}\right)^{6}\right]$$

$$V_{EL} = \frac{1}{2}\sum_{i,j,i\neq j} \frac{q_i q_j}{R_{ij}}$$

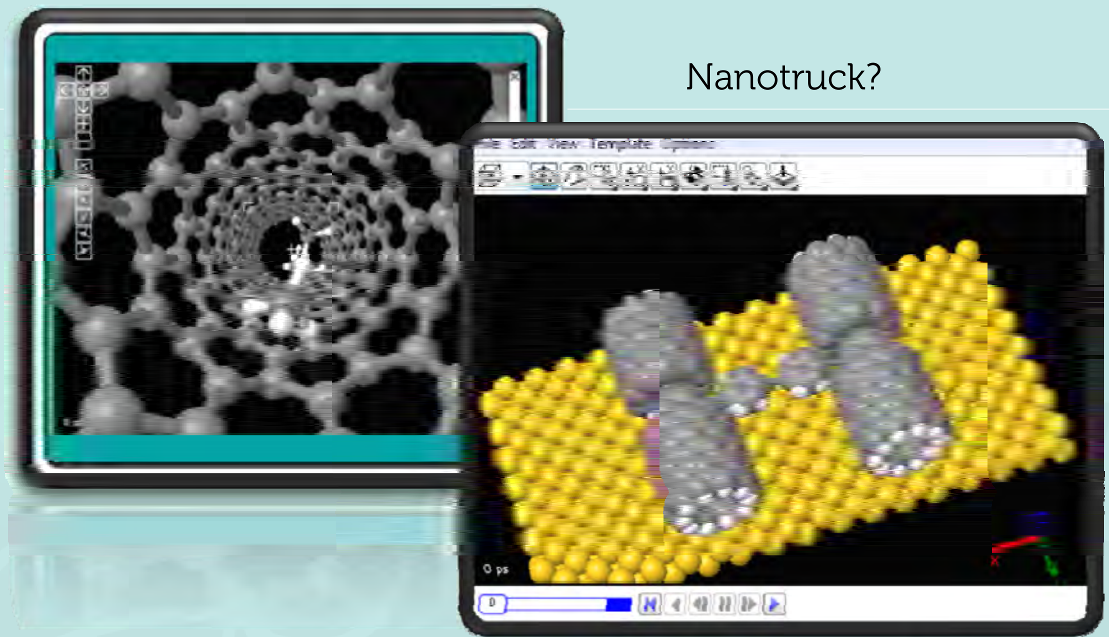
$$V_{BS} = \frac{1}{2}\sum_{m\in bonds} k_m^l (l_m - l_m^0)^2$$

$$V_{AB} = \frac{1}{2}\sum_{m\in angles} k_m^\theta (\theta_m - \theta_m^0)^2$$

$$V_{PT} = \frac{1}{2}\sum_{m\in torsions} V_m [1 + \cos(n_m \omega_m - \gamma_m)]$$

$$V_{IT} = \frac{1}{2}\sum_{m\in torsions} k_m^\xi (\xi_m - \xi_m^0)^2$$

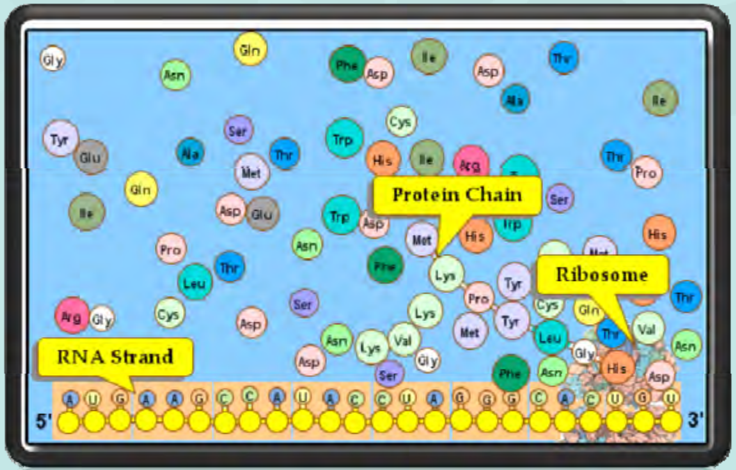
Water molecules in a carbon nanotube



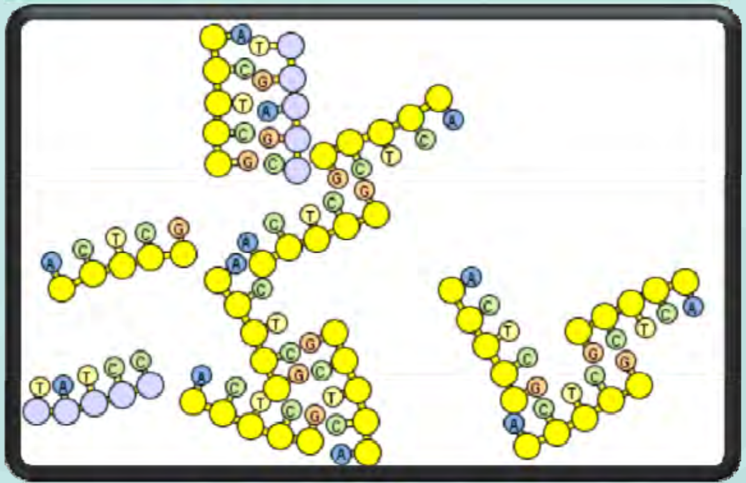
Nanotruck?

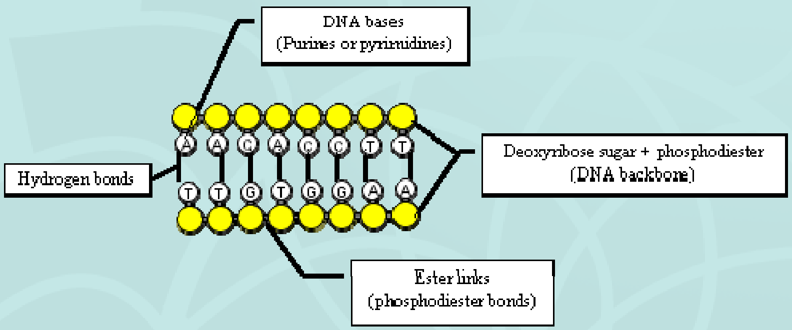
Coarse-Grained Particle Dynamics

a) A coarse-grained simulation of **translation** (making proteins from messenger RNA). Each amino acid, RNA base, and RNA backbone are represented by a particle. The amino acids randomly bounce into the ribosome site and the one that matches the current RNA triplet will be attached to the growing polypeptide. The solvent is not explicitly modeled.

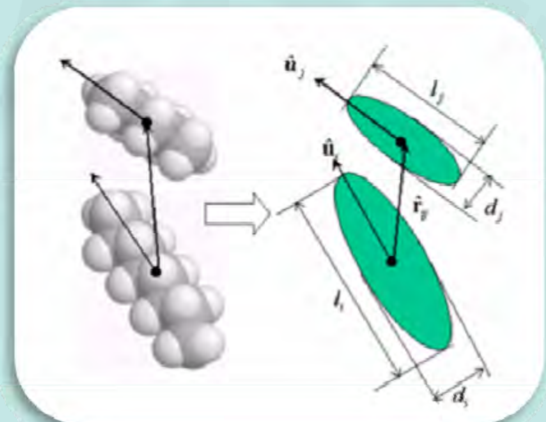


b) **DNA hybridization**, which makes use of base pairing between nucleotides of short denatured DNA strands, is responsible for biotechnologies such as Southern blot and DNA microarrays.



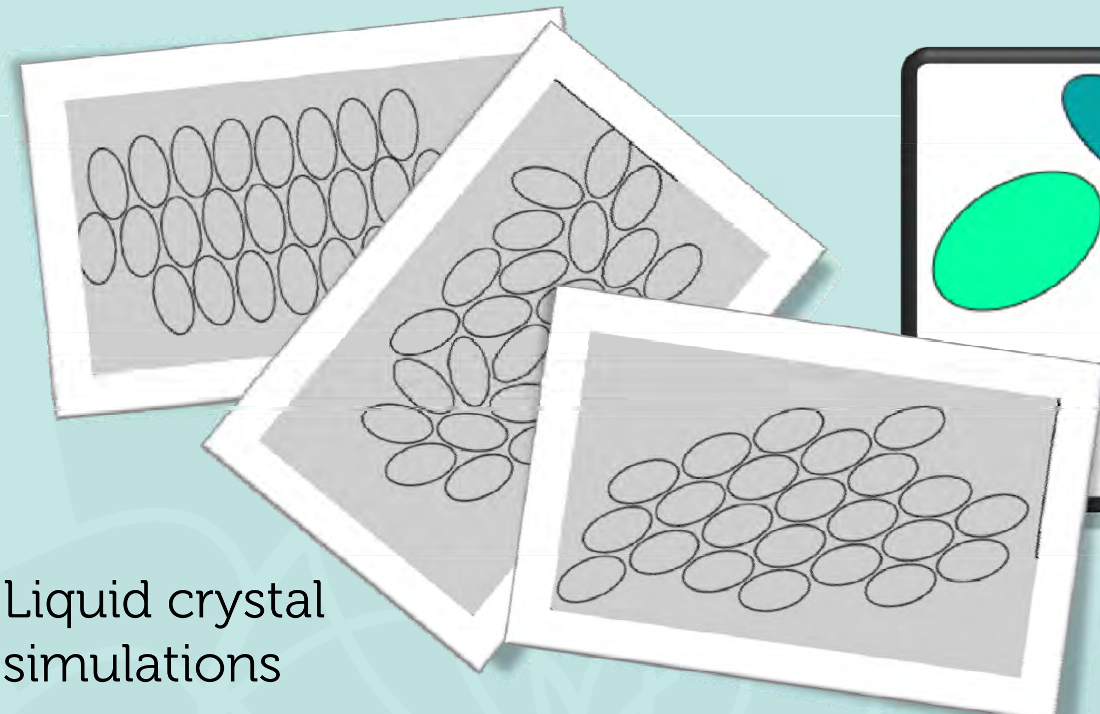


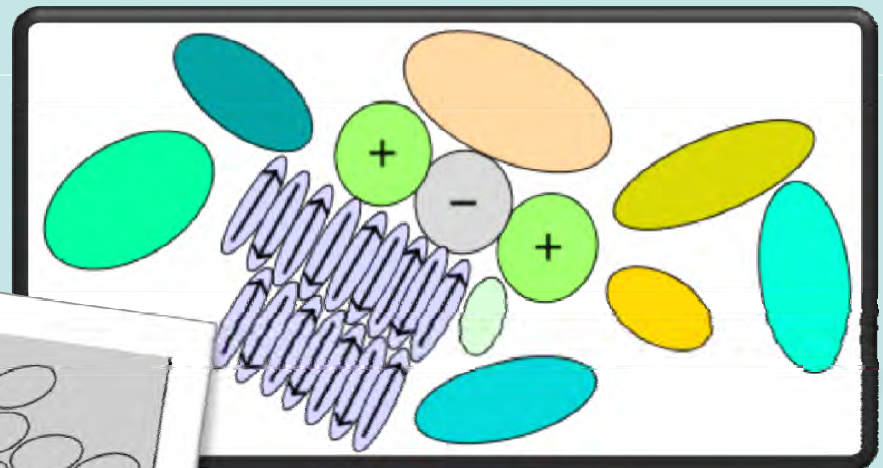
Gay-Berne Molecular Dynamics



Interaction potential between ellipsoids

$$V_{GB} = \sum_{i}\sum_{j>i} 4\varepsilon(\hat{u}_i,\hat{u}_j,\hat{r}_{ij})\left\{\left[\frac{\sigma_0}{r_{ij}-\sigma(\hat{u}_i,\hat{u}_j,\hat{r}_{ij})+\sigma_0}\right]^{12} - \left[\frac{\sigma_0}{r_{ij}-\sigma(\hat{u}_i,\hat{u}_j,\hat{r}_{ij})+\sigma_0}\right]^{6}\right\}$$
$$+\sum_{i}\sum_{j>i}\frac{q_i q_j}{r_{ij}} + \sum_{i}\sum_{j>i}\frac{q_i q_j}{r_{rij}^2}\left(q_j p_i \hat{u}_i\cdot\hat{r}_{ij} + q_i p_j \hat{u}_j\cdot\hat{r}_{ij}\right)$$
$$+\sum_{i}\sum_{j>i}\frac{p_i p_j}{r_{ij}^3}\left[\hat{u}_i\cdot\hat{u}_j - 3(\hat{u}_i\cdot\hat{r}_{ij})(\hat{u}_j\cdot\hat{r}_{ij})\right]$$

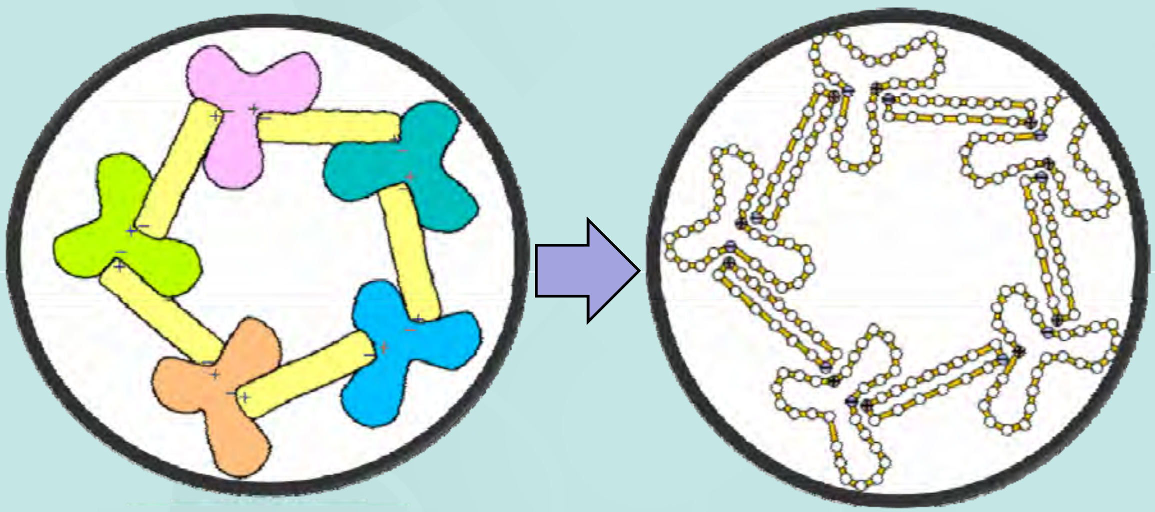


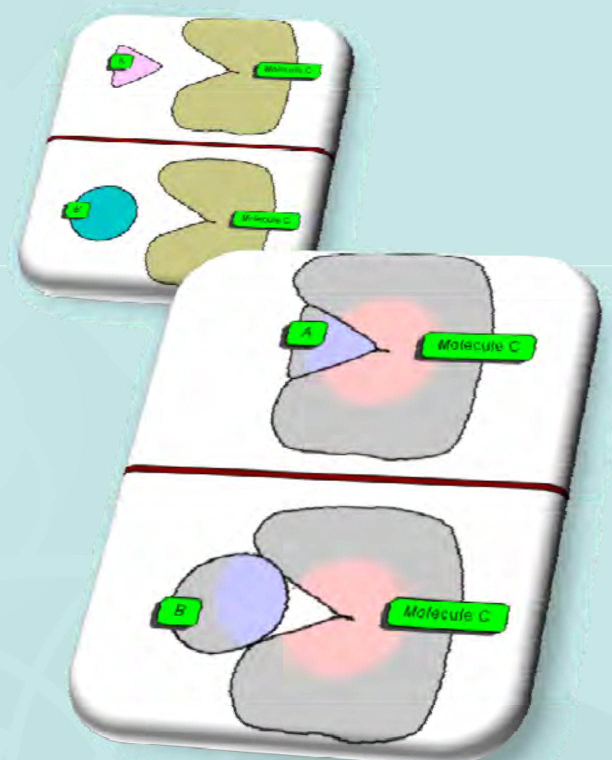


Liquid crystal simulations

Soft-Body Dynamics

A flexible body is discretized into
a particle chain model joined by elastic forces
with van der Waals surface and partial electric charges.



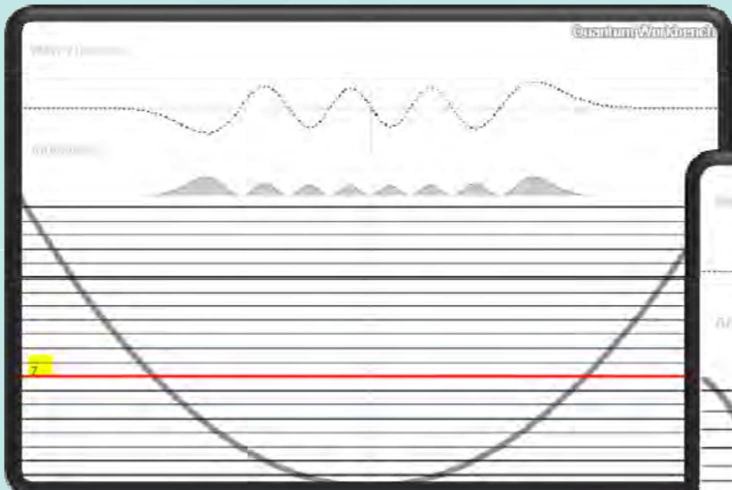


Protein-ligand binding

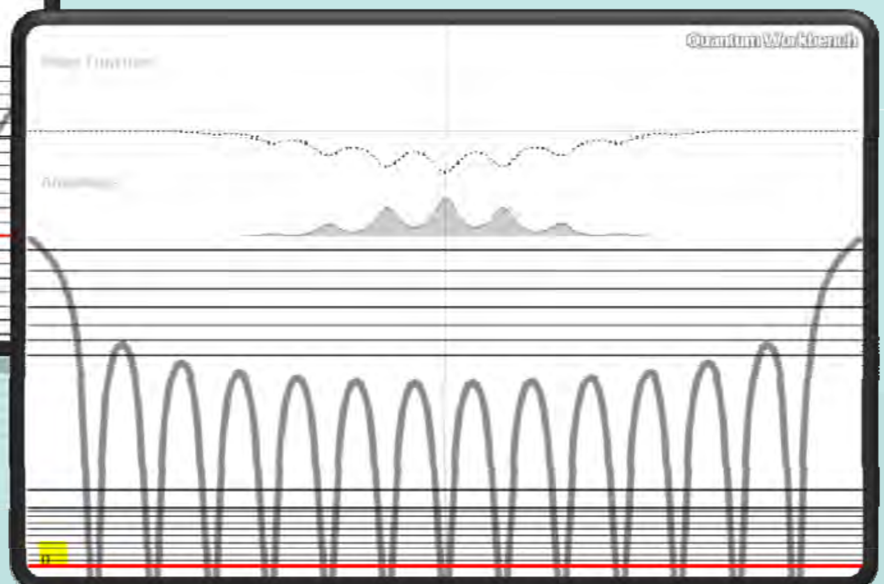
Stationary State Quantum Mechanics

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r)+V(r)\psi(r)=E\psi(r)$$

Quantum harmonic oscillator



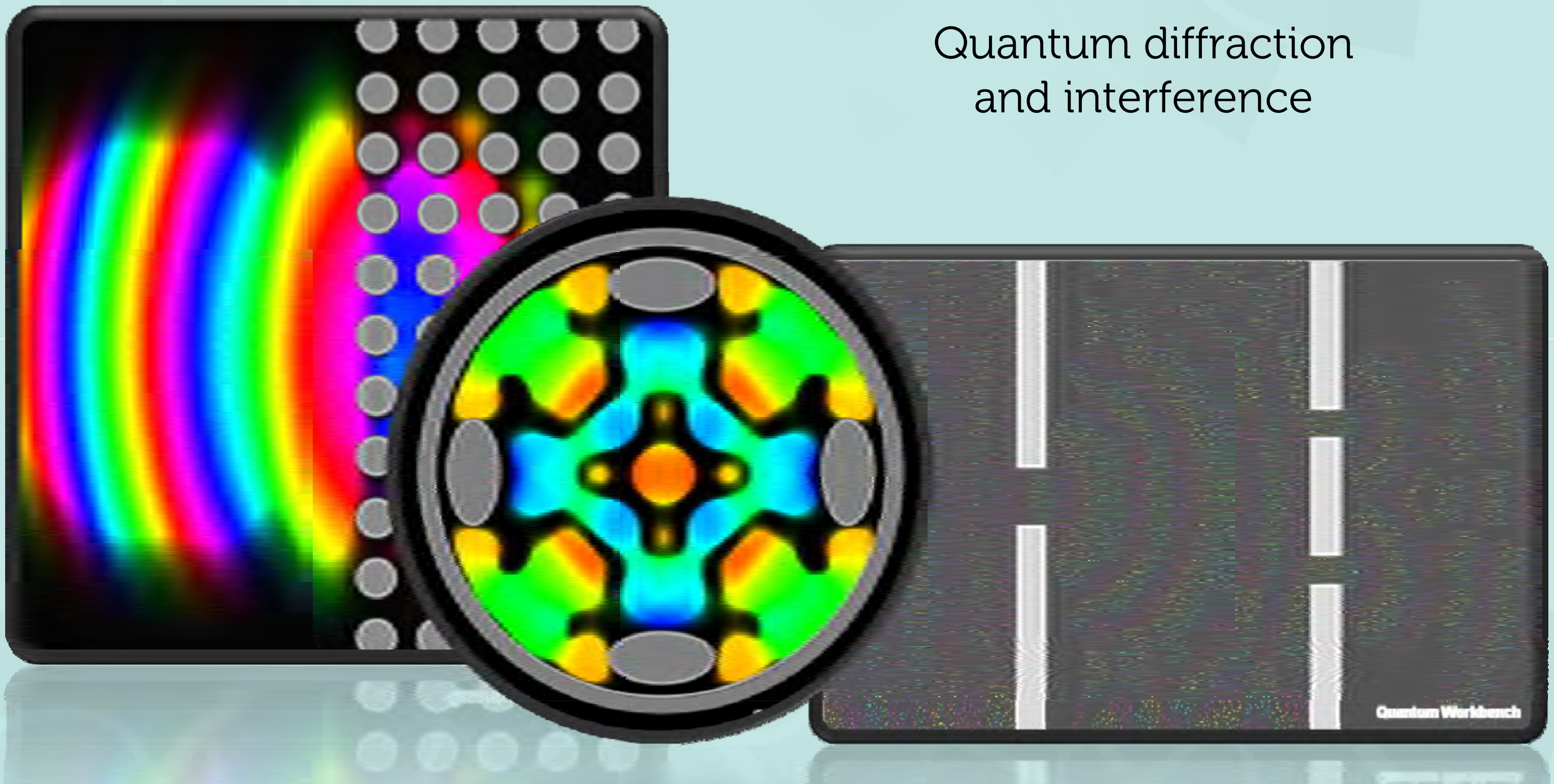
Quantum states in crystal lattice



Quantum Dynamics

$$i\hbar \frac{\partial}{\partial t}\psi(r,t) = -\frac{\hbar^2}{2m}\nabla^2\psi(r,t) + V(r)\psi(r,t)$$

Quantum diffraction
and interference

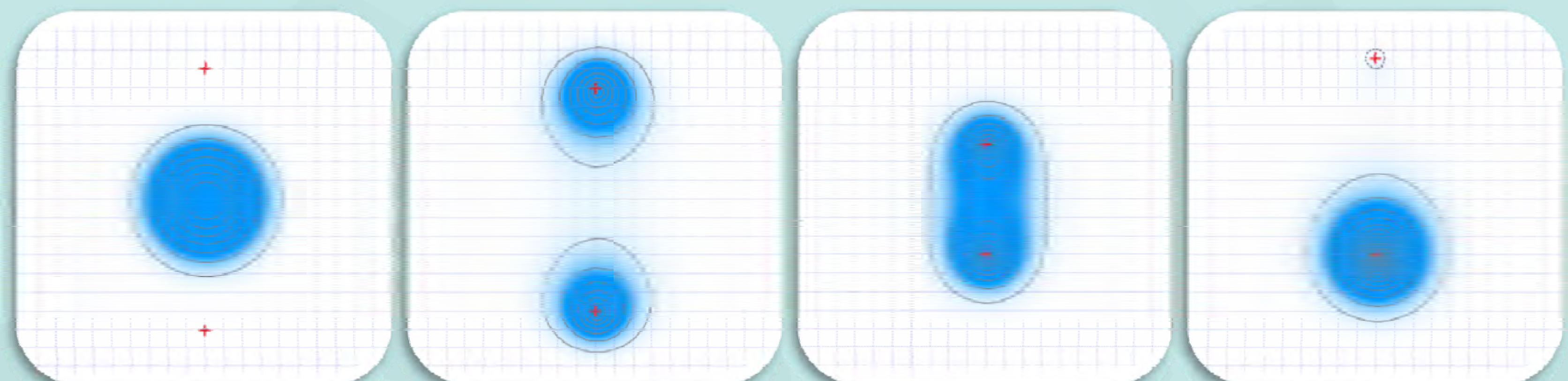


Imaginary Time Quantum Dynamics

$$i\hbar\frac{\partial}{\partial t}\psi(r,t) = -\frac{\hbar^2}{2m}\nabla^2\psi(r,t) + V(r)\psi(r,t) \xrightarrow{t=-i\tau} -\hbar\frac{\partial}{\partial \tau}\psi(r,\tau) = -\frac{\hbar^2}{2m}\nabla^2\psi(r,\tau) + V(r)\psi(r,\tau)$$

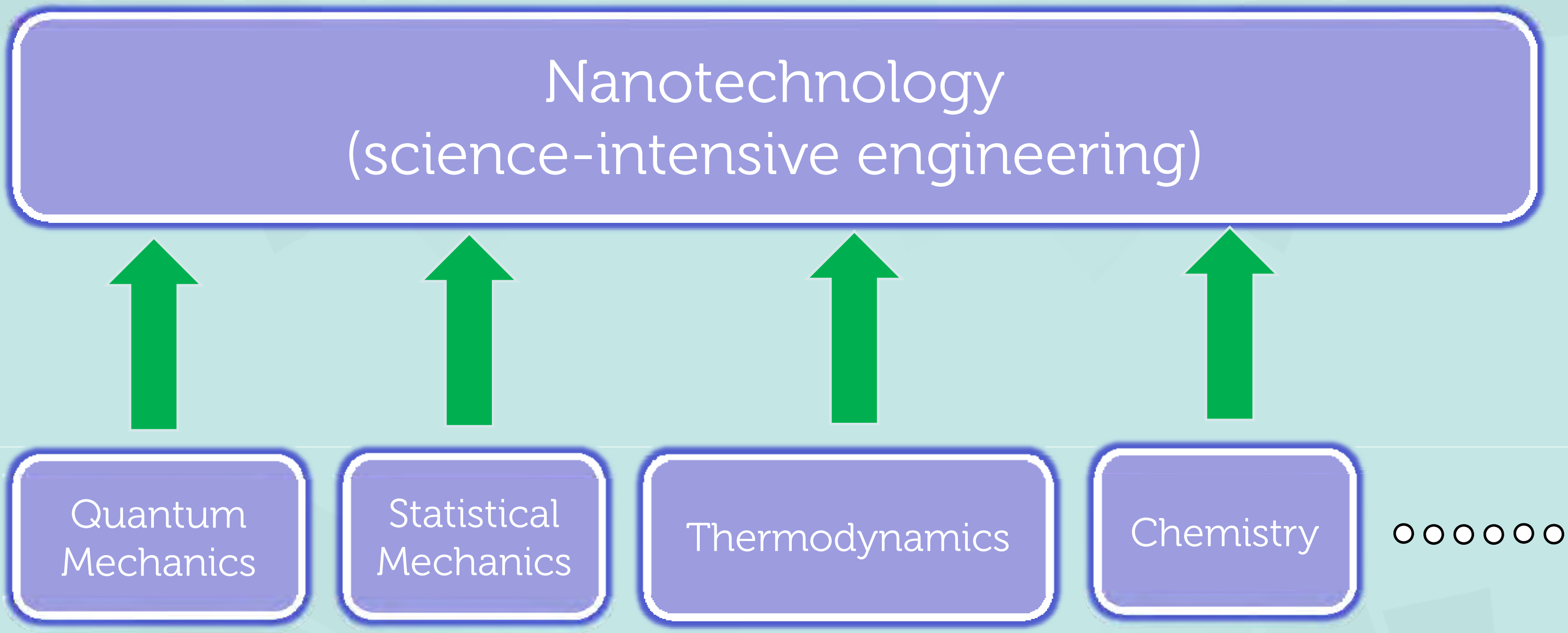
Drag and drop to discover possible states of a 2D quantum system.

Two protons and an electron cloud.	Two H atoms polarized by each other (the origin of the van der Waals force).	An H_2 hydrogen molecule when the electron cloud overlaps significantly.	A H anion (H^-) and a proton.



Teaching nanotechnology with simulations

Use visual simulations to teach the science foundation of nanotechnology



E. Drexler, How to study for a career in nanotechnology, 2/26/2010
http://www.nanowerk.com/spotlight/spotid=15067.php

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Basic science of electrons, atoms, and molecules

Visual simulations

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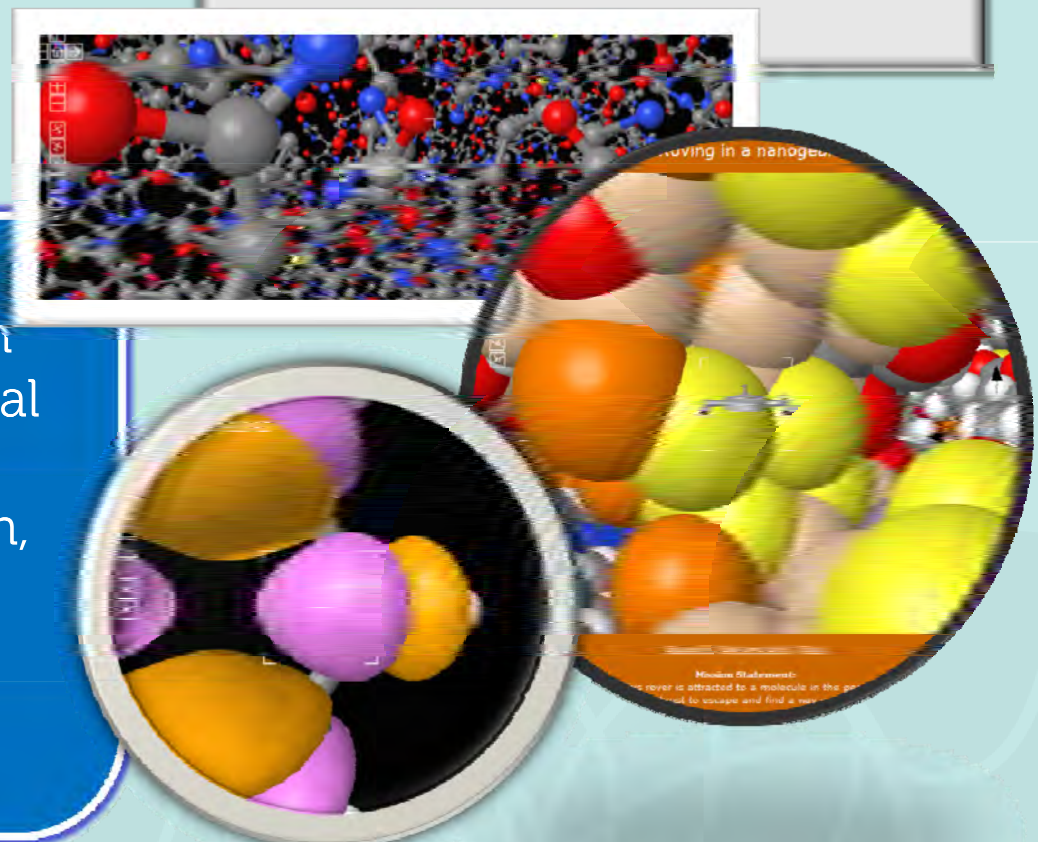
Virtual atomic microscopes for viewing into the nanoscopic world and exploring these concepts.



Fundamental concepts such as atomic structure, chemical bonding, interatomic interactions, thermal motion, and so on are the building blocks of nanoscience and nanotechnology.

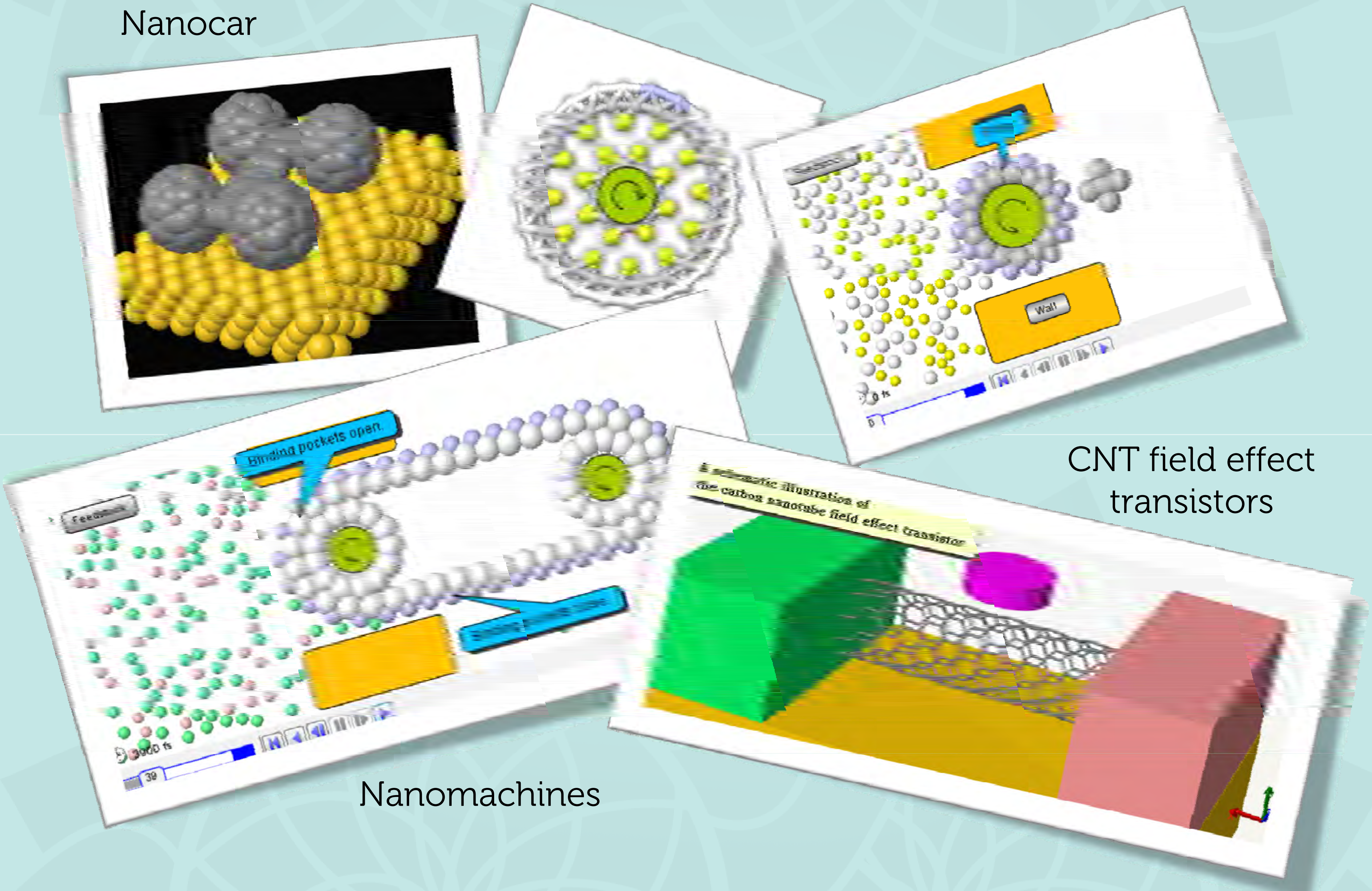
Use visual simulations in nanotechnician education: What can be done?

- Convey the visions of nanotechnology
- Explain the scientific principle of a technology
- Simulate a laboratory procedure

⋮

Convey the visions of nanotechnology

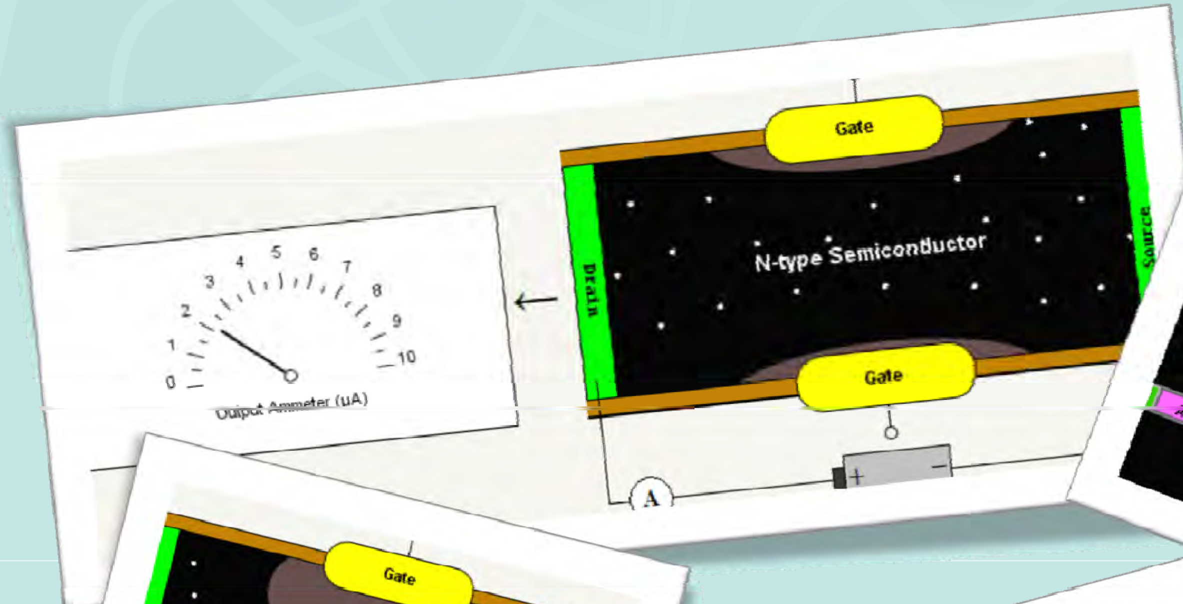
Nanocar



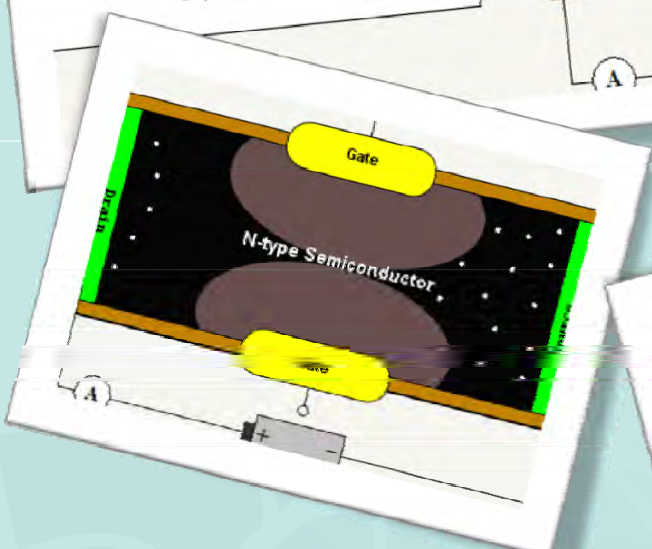
CNT field effect transistors

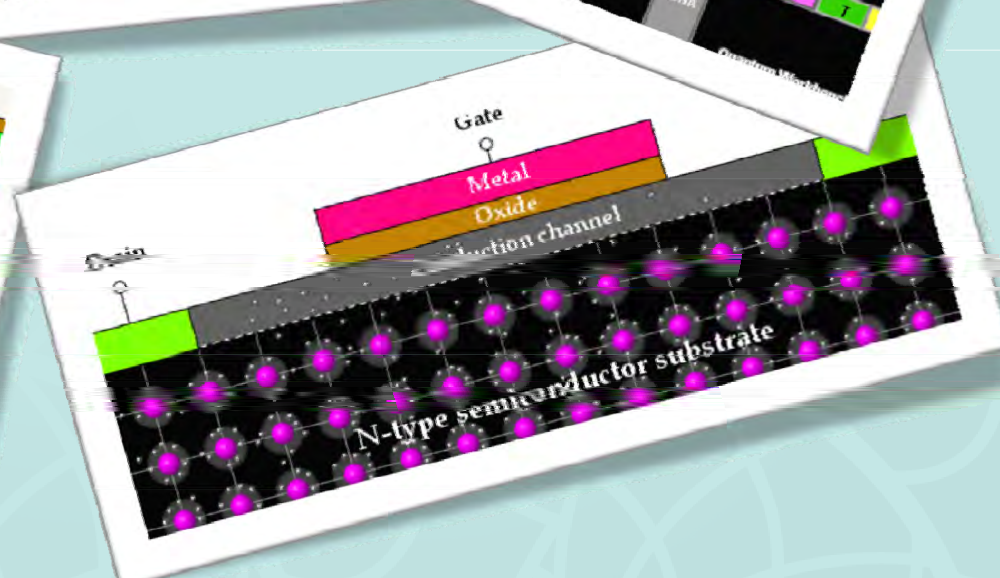
Nanomachines

Explain the scientific principle of a technology



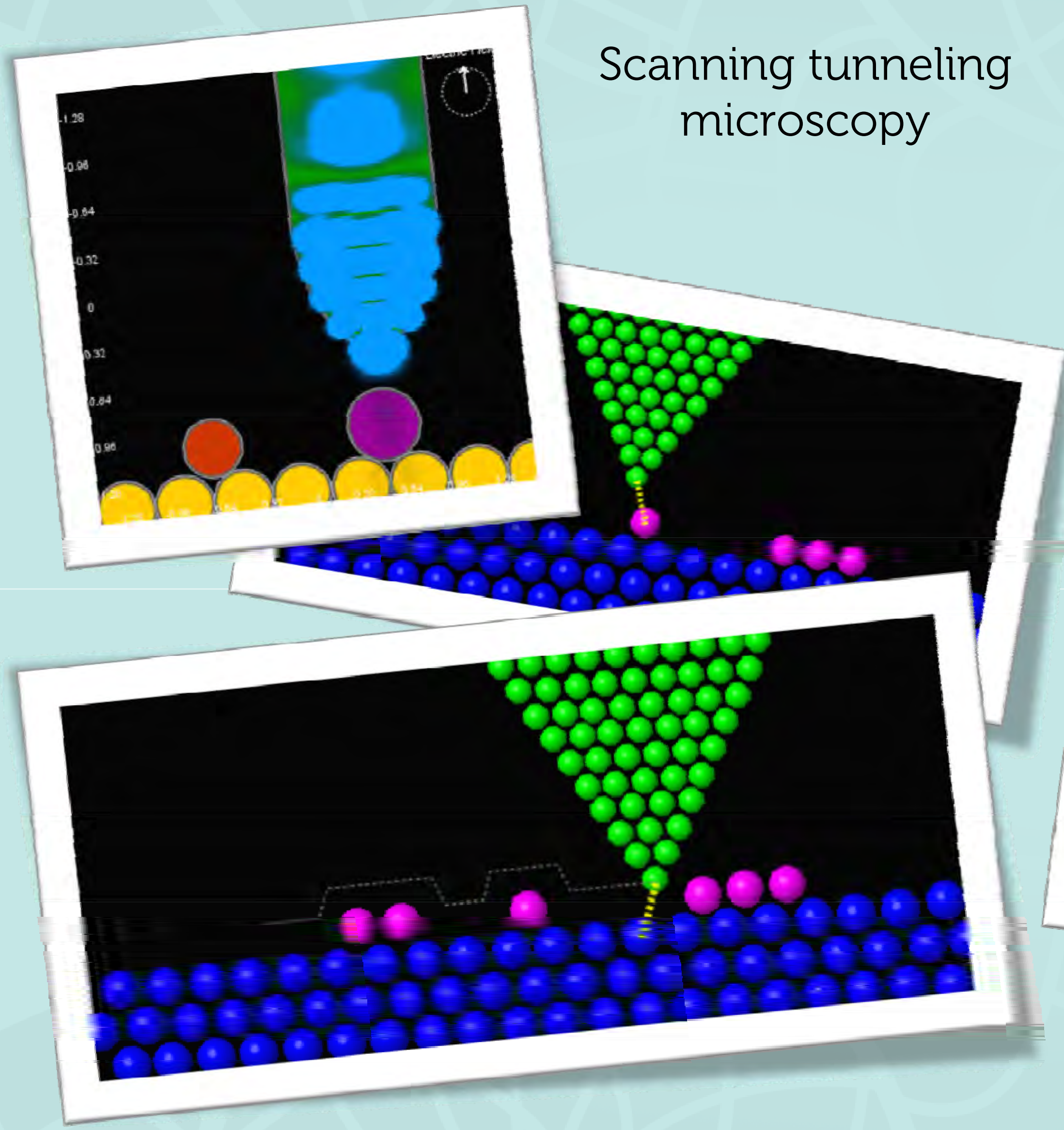
Nanopore DNA sequencing



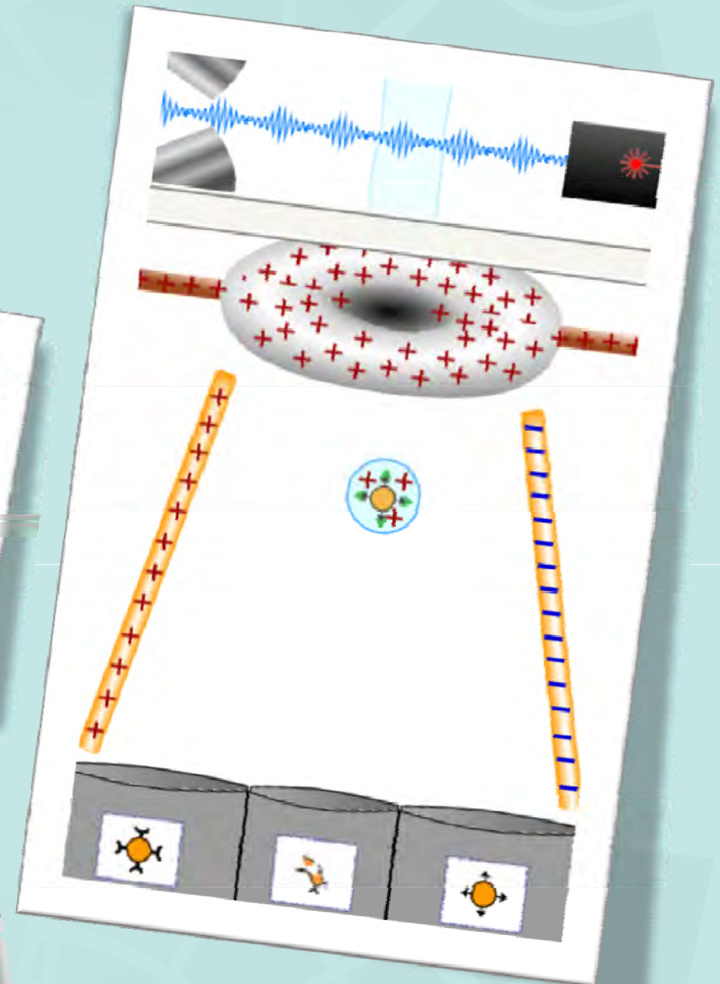


Field effect transistors

Simulate a laboratory procedure



Scanning tunneling microscopy



Fluorescence activated cell sorting

Conclusions & discussions

1) A better than "better than nothing" solution to grassroots K-14 nanotechnology education?
2) Evidence-based best strategies to use visual simulations in the classroom?
3) Deceptive clarity of visual simulations (watching and playing without learning)?
4) Mixed-reality to connect simulations to the real world through sensors?

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Nano-Link Midwest Regional Center for Nanotechnology Education

Thank you!