

Predicting Structures and Properties of Nano-scale Materials

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Why do we need to predict the structures and properties of nano-scale materials ?

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How do we predict the structures and the properties of nanostructures?

Methodology —

- **First Principles Simulations:** Density functional theory (DFT)-based methods (small size/short time) (VASP, WIEN2K, etc.)
- **Semi-empirical Simulations:** Non-orthogonal tight-binding methods (larger size/longer time)
- **Semi-empirical simulations:** Self-consistent and environment-dependent (SCED) approach (larger size/longer time) (*Phys. Rev. B* 74, 155408 (2006))

	<i>Ab initio</i> methods	Semi-empirical methods	Classical simulations
Major features	Have predictive power but have limitation on the size of the system	Address problems that are beyond the scope of <i>ab-initio</i> ; may have transferability issues	Simulations of large systems possible- but poor predictive power
Major features	Electronic band structure Calculations required		Electronic band structure not required
Hamiltonian	Parameter free	Parameterized Functions used for the Hamiltonian	Parameterized inter- atomic Potential functions
Software	Gaussian, VASP, WIEN2K, SIESTA, ABINIT, CPMD, etc.	Gaussian, CHSSI-PET, Ames Lab, NRL Group	CHARMM, AMBER, DISCOVER

Methodology

Quantum Mechanical Simulations



accurate, reliable, and robust results, and therefore have the predictive power

Ø Schrödinger equation for **many-electron** systems in the external ionic field:



$$H \psi = E \psi$$

$$H = -\sum_i \frac{\hbar^2}{2m} \nabla_i^2 + \sum_{i,j} v(\vec{r}_i, \vec{R}_j) + \sum_{i,j} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|} ; \quad (\vec{r}_1, \dots, \vec{r}_n)$$

Ø Schrödinger equation in the **one-electron** approximation (in an effective potential)



$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_{eff} \right) \psi = E \psi$$

● First principles simulations

Density Functional Theory (DFT) — Kohn-Sham Equations:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{eff}} \right) \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r})$$

DFT with Local Density Approximation (LDA):

$$V_{\text{eff}} = V_{\text{eff}}(\mathbf{r})$$

or

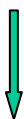
DFT with Generalized Gradient Approximation (GGA):

$$V_{\text{eff}} = V_{\text{eff}}(\mathbf{r}, \nabla \rho(\mathbf{r}))$$

$$E^{\text{total}} = \sum_i^{\text{occ}} \epsilon_i - \frac{e^2}{2} \iint d^3r d^3r' \frac{\rho(\mathbf{r}) \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + E_{\text{xc}}[\rho] = \int d^3r \epsilon_{\text{xc}}(\mathbf{r}) \rho(\mathbf{r})$$



<http://cms.mpi.univie.ac.at/vasp/vasp.html>



Ø A complex package for performing *ab-initio* quantum-mechanical molecular dynamics (**MD**) simulations using a **plane wave basis set**.

Ø DFT-based method using either **LDA** or **GGA** for exchange-correlation energy.

Ø The interaction between ions and electrons is described by **ultra-soft Vanderbilt pseudopotentials** or by the projector-augmented wave method.

high reliability and reputation, and is considered to have the predictive power !

!! Limitations in DFT-based ab initio simulations

- Ø The diagonalization and the calculation of the Hamiltonian matrix elements **go as N^3** .
- Ø DFT-based simulations are applicable only for systems of **no more than a few hundreds of atoms**.
- Ø The time scale available for the molecular dynamics study **only reaches picoseconds**.
- Ø These limitations will **prevent first-principles simulations** from applications to complex chemical reactions, biological systems or nanostructures with low or no symmetry.

• Semi-empirical simulations

Two-Center Non-Orthogonal Tight-Binding (NOTB) Eigenvalue Equation:

$$\begin{matrix} \langle n | H | m \rangle & c_m \\ \langle n | H | m \rangle & H_{nm} \\ \langle n | m \rangle & S_{nm} \end{matrix} \left. \vphantom{\begin{matrix} \langle n | H | m \rangle \\ \langle n | H | m \rangle \\ \langle n | m \rangle \end{matrix}} \right\} \text{Parameterized functions} \quad ; \quad c_n$$

Ø Two key advantages: (1) capturing the **quantum nature** of the problem; (2) increasing both the size and the time of simulation by **about two orders** of magnitude.

Ø A system-specific tool: the **transferability** of the NOTB Hamiltonian is crucially dependent on the parametric functions defining the Hamiltonian.

!! Disadvantage of the NOTB Hamiltonians: limitation of the transferability

Ø They include only **two-center interactions** and they have no framework to allow the **self-consistent** determination of the charge re-distribution and the **environment-dependent** multi-center interactions. These are two key ingredients for an appropriate description of **bond-breaking** and **bond-forming** processes.

Ø They are **not equipped** to determine the equilibrium configuration of systems such as nanostructures where these **two processes are dominant**. Thus they **do not have the predictive power** and can only be used, in the strictest sense, to provide **explanation** for system-specific experimental results.

Development of new semi-empirical Hamiltonian at CMT group of UofL

Self-Consistent and Environment-Dependent Hamiltonian in the framework of Linear Combination of Atomic Orbitals



SCED-LCAO

$$\begin{aligned}
 & \left(\begin{matrix} i & |H| & j \\ c_i & & c_j \end{matrix} \right) \xrightarrow{\text{LCAO}} N_i^{occ} \left(\begin{matrix} c_i & c_j \end{matrix} \right) f S_{i,j} \\
 & \left(\begin{matrix} i & |H| & j \\ c_i & & c_j \end{matrix} \right) \xrightarrow{\text{LCAO}} H_{i,j}^{SCED\ LCAO}(N_i, N_j, \{V_{ki}^N\}, \{V_{kj}^N\}, \{V_{ki}^Z\}, \{V_{kj}^Z\}) \\
 & \text{LCAO} \quad c_i \quad AO_i
 \end{aligned}$$

Phys. Rev. B 74, 155408 (2006)



Materials simulations based on the SCED-LCAO Hamiltonian are reliable, transferable, robust, and has the predictive power!

Construction of the SCED- LCAO Hamiltonian:

Hamiltonian matrix element:

$$H_{i,j}^{SCED \text{ LCAO}} = \frac{1}{2} \underbrace{\{K(R_{ij})(\psi_i, \psi_j)\}}_{\text{Two-center interactions}} \underbrace{[(N_i, Z_i)U_i, (N_j, Z_j)U_j]}_{\text{Treatment of charge re-distribution}} + \underbrace{\sum_k \{[(N_k V_N(R_{ik}), Z_k V_Z(R_{ik})) (N_k V_N(R_{jk}), Z_k V_Z(R_{jk}))]\} S_{i,j}(R_{ij})}_{\text{Environment-dependent multi-center interactions}}$$

Parametric functions:

$K(R_{ij}) = e^{-\kappa R_{ij}}$	(Scaling function)
$S_{ij} = (A + B R_{ij}) \frac{[1 - e^{-d R_{ij}}]}{[1 - e^{-(d + R_{ij})}]}$	(Overlap matrix element)
$V_N(R_{ik}) = V_Z(R_{ik}) = V_N(R_{ik})$	(Potential function of electron-electron interaction)
$V_Z(R_{ik}) = \frac{E_0}{R_{ik}} \{1 - (1 - B_Z R_{ik}) e^{-z R_{ik}}\}$	(Potential function of electron-ion interaction)
$V_N = (A_N + B_N R_{ik}) \frac{[1 - e^{-N d_N}]}{[1 - e^{-N(d_N + R_{ik})}]}$	(Short-range potential function)

Framework of Establishing a Semi-Empirical Hamiltonian Possessing Predictive Power

$$i \mid H \mid j \quad c_i \quad c_i \quad i \mid j$$

$$i \mid H \mid j \quad H_{i,j}^{SCED \ LCAO}$$

$$i \mid j \quad S_{i,j}$$

} Parameterized functions



Transferability

Physical properties in small clusters, bulk phases, band-structures, etc.

Fitting

Corresponding *ab initio* calculations and/or experimental results



Robustness








Physical properties in more complicated structures







Comparing

Corresponding *ab initio* calculations and/or experimental results

Transferability of the SCED-LCAO Hamiltonian

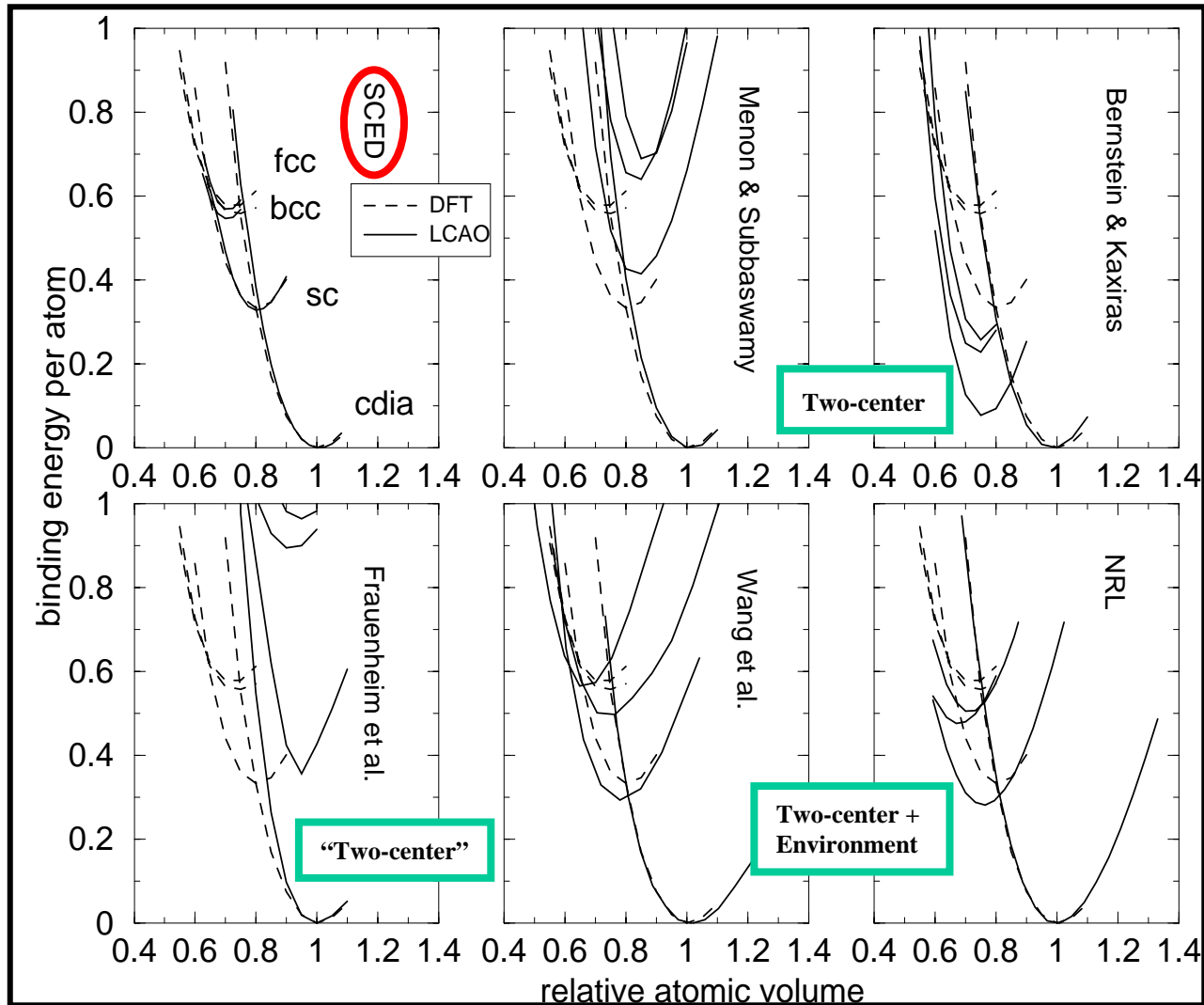
Fitting results on small Si clusters

Cluster	Symmetry	Present work	<i>ab initio</i> values ^a
SiB _{2B}	DB _{ihB} 	2.226 Å -2.435 eV	2.288 Å -2.499 eV
SiB _{3B}	CB _{2vE} 	2.284 Å 2.168 Å -3.413 eV	2.357 Å 2.158 Å -3.575 eV
SiB _{3B}	DB _{ihB} 	2.141 Å -3.427 eV	2.167 Å -3.404 eV
SiB _{4B}	DB _{2I} 	2.275 Å -4.101 eV	2.311 Å -4.242 eV
SiB _{4B}	TB _{dE} 	2.332 Å -3.773 eV	2.474 Å -3.659 eV
SiB _{4B}	DB _{ih-} 	2.116 Å 2.164 Å -3.289 eV	2.156 Å 2.176 Å -3.364 eV
SiB _{5B}	DB _{3I} 	2.207 Å 3.141 Å -4.526 eV	2.306 Å 3.064 Å -4.453 eV

Cluster	Symmetry	Present work	<i>ab initio</i> values ^a
SiB _{5B}	CB ₄ 	2.209 Å 2.358 Å -4.327 eV	2.275 Å 2.513 Å -4.266 eV
SiB _{5B}	DB _i 	2.082 Å 2.128 Å -3.545 eV	2.133 Å 2.144 Å -3.534 eV
SiB _{5B}	TB _d 	2.127 Å 3.475 Å -3.334 eV	2.215 Å 3.617 Å -3.283 eV
SiB _{6B}	DB _{4hB} 	2.248 Å 2.639 Å -4.698 eV	2.363 Å 2.734 Å -4.664 eV
SiB _{6B}	DB _{3dR} 	2.261 Å 2.948 Å -3.896 eV	2.285 Å 3.208 Å -3.972 eV
SiB _{6B}	DB _{ihR} 	2.057 Å 2.072 Å 2.149 Å -3.446 eV	2.098 Å 2.134 Å 2.158 Å -3.446 eV

a. Gaussian 98 MPW1PW91/cc-pVTZ.

Fitting results on the phase diagram of bulk Si



The SCED-LCAO approach with the inclusion of explicit self-consistency and environment-dependence represents the most complete package to capture the environment-dependent screening effects under various local configurations.

Physical properties of bulk Si (diamond phase)

Properties	SCED-LCAO	Other TB	DFT	Expt.
Lattice constant (Å)	5.443	5.426 ^e ; 5.399 ^f ; 5.427 ^g ; 5.417 ^h	5.451 ^a ; 5.399 ^f	5.429 ^b
Cohesive energy (eV/atom)	4.904	4.71 ^f ; 5.19 ^g ; 4.97 ^h	4.67 ^a ; 4.70 ^f	4.63 ^c
Bulk Modulus (GPa)	96.6	108.3 ^e ; 104.8 ^f ; 153.5 ^g ; 115.1 ^h	98 ^a ; 96.4 ^e ; 98 ^f	99 ^d
C ₁₁ (GPa)	166.3	179 ^e ; 145 ^f ; 218 ^g ; 185 ^h	152 ^e	166 ^d
C ₁₂ (GPa)	61.7	73 ^e ; 84.5 ^f ; 121 ^g ; 80.1 ^h	60 ^e	64 ^d
C ₄₄ (GPa)	93.7	95 ^e	101 ^e	80 ^d

a: Phys. Rev. B**26**, 5668 (1982).

b: *The Structure of Elements* (Wiley, New York, 1974).

c: *Atomic Energy Levels* (National Bureau of Standards, Washington, D.C., 1949 (Circular No. 467, Vol. I)).

d: J. Appl. Phys. **24**, 988 (1953); **34**, 651 (1963); **35**, 2161 (1964).

e: Phys. Rev. B**62**, 4477 (2000).

f: Phys. Rev. B**56**, 10488 (1997).

g: Phys. Rev. B**55**, 9231 (1997); **47**, 12754 (1993); **50**, 11577 (1994).

h: Phys. Rev. B**52**, 11492 (1995).

Showing definitely the reliability of the SCED-LCAO Hamiltonian for Si

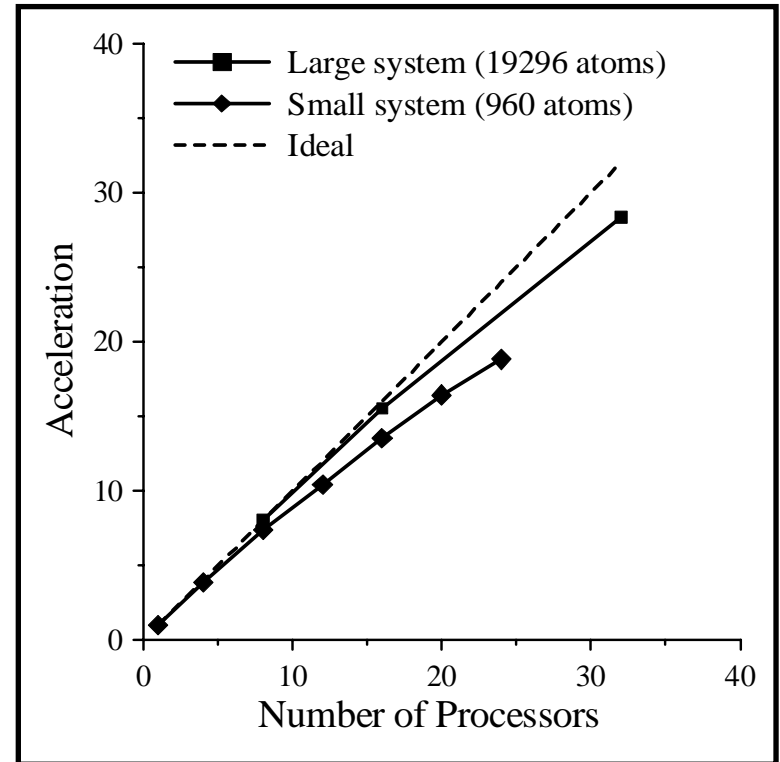
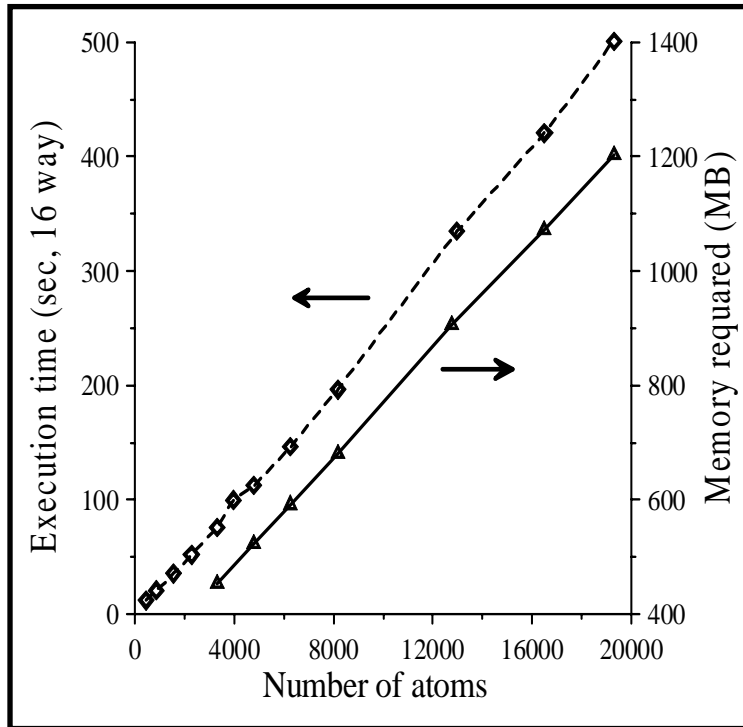
Efficiency of the SCED-LCAO approach

Computational speed and memory usage (testing on Si₇₁ cluster)

Method	Execution time	Memory
VASP	~ 189 h 22 m 33 s	~ 300 MB
SCED-LCAO	~ 6 h 55 m	~ 63.4 MB

The **SCED-LCAO** approach is about **30 times faster** than VASP, and requires about **five times less memory** for the relaxation of a Si₇₁ cluster.

Implementation of the order- N scheme on top of the SCED-LCAO Hamiltonian for large-scale systems (testing on Si NWs)



The advantages of **Order- N scheme** (C.S. Jayanthi, et al, *PRB*, 57, 3799 (1998)):

- (1) **linear scaling** with the size of the system;
- (2) **easy to develop its efficient parallelized version**, which allows for the investigation of systems of **up to tens of thousands of atoms** and approaches **two or three orders of magnitude speed up** for those systems as compared to VASP.

The features of the SCED-LCAO Hamiltonian formulation

SCED-LCAO

$$\begin{array}{c}
 \begin{array}{ccccccc}
 i & |H| & j & c_i & c_i & i & |j \\
 \uparrow & & & & & & \rightarrow N_i^{ooc} \\
 & & & & & & c_i c_j f S_{i,j} \\
 & & & & & & \downarrow \\
 i & |H| & j & H_{i,j}^{SCED\ LCAO}(N_i, N_j, \{V_{ki}^N\}, \{V_{kj}^N\}, \{V_{ki}^Z\}, \{V_{kj}^Z\}) \\
 & & & \downarrow \\
 & & & c_i^{LCAO} \quad c_i^{AO}
 \end{array}
 \end{array}$$

Ø **Overcoming** the major drawback of other semi-empirical Hamiltonians in terms of the **transferability**.

Ø The physical content for terms in the parameterized functions also makes it possible to **track properties** of the system under consideration to their underlying physics.

Ø Based on the implementation of order- N scheme, the **SCED-LCAO** approach allows **quantum mechanics-based** simulations for **large-scale complex** nanostructures that are beyond the scope of DFT-based simulations.

Demonstration of the robustness of the SCED-LCAO Hamiltonian

— Studies on Si-based systems —

- **0-dimensional system:** The stable structure of Si_{71} cluster
- **1-dimensional system:** The morphology of Si nanowires
- **2-Dimensional system:** The reconstruction of Si (001) surface and the energy landscape of a Si monomer adsorbed on the reconstructed Si (111) -7x7 surface

THE FUTURE

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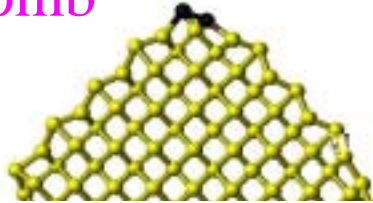
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* H . 121
 12- . 122

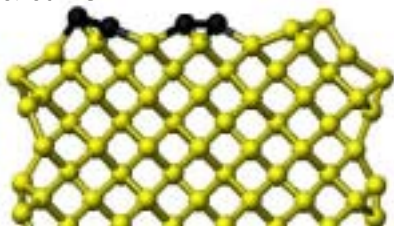
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Morphology of Silicon $\langle 001 \rangle$ nanowires

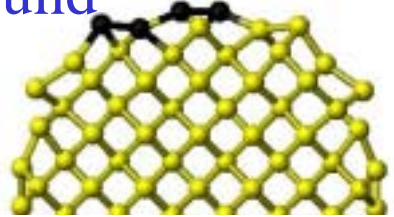
“rhomb”



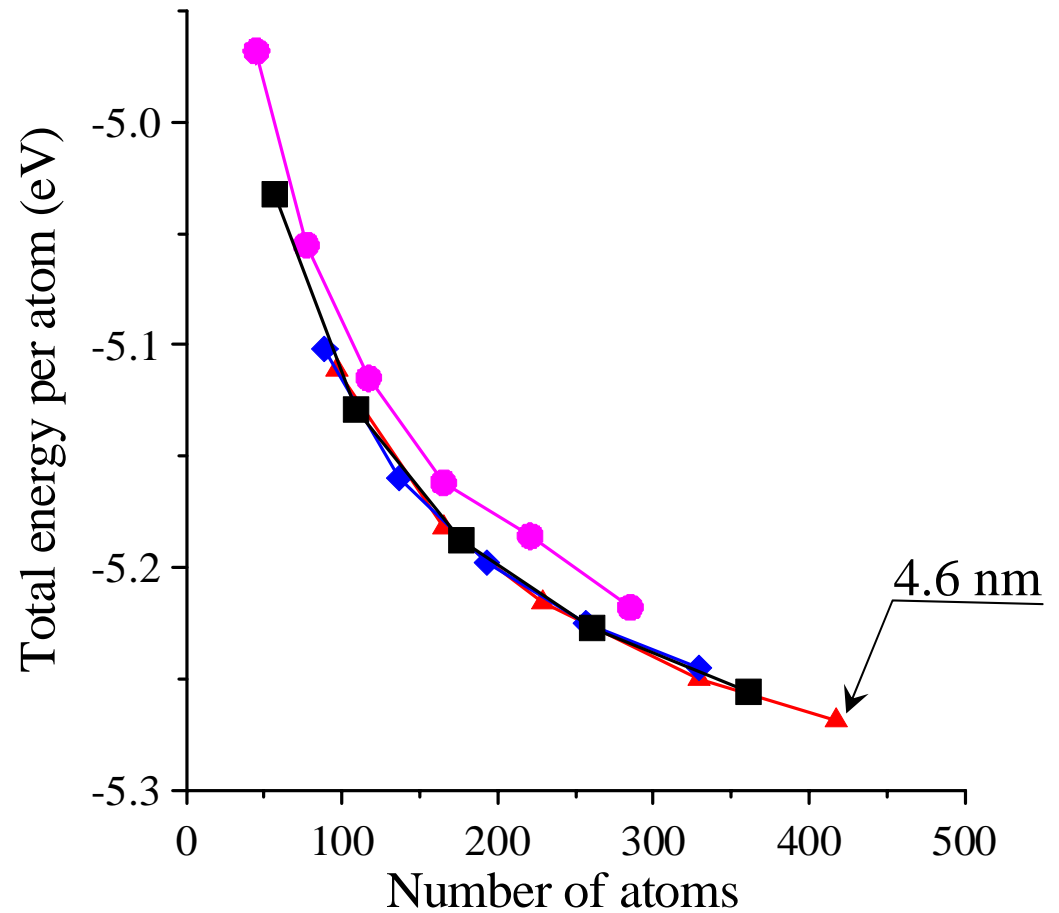
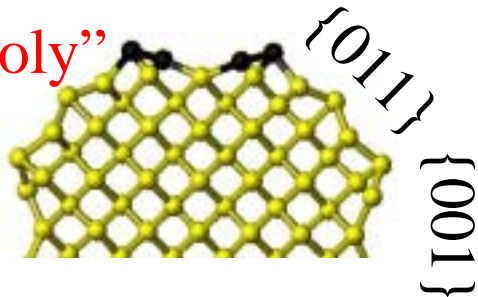
“square”

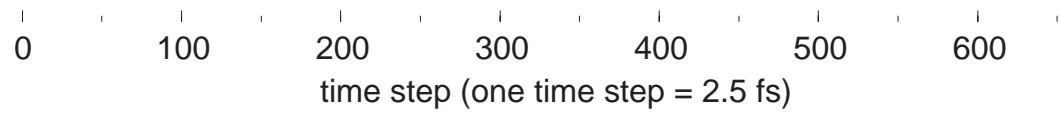


“round”



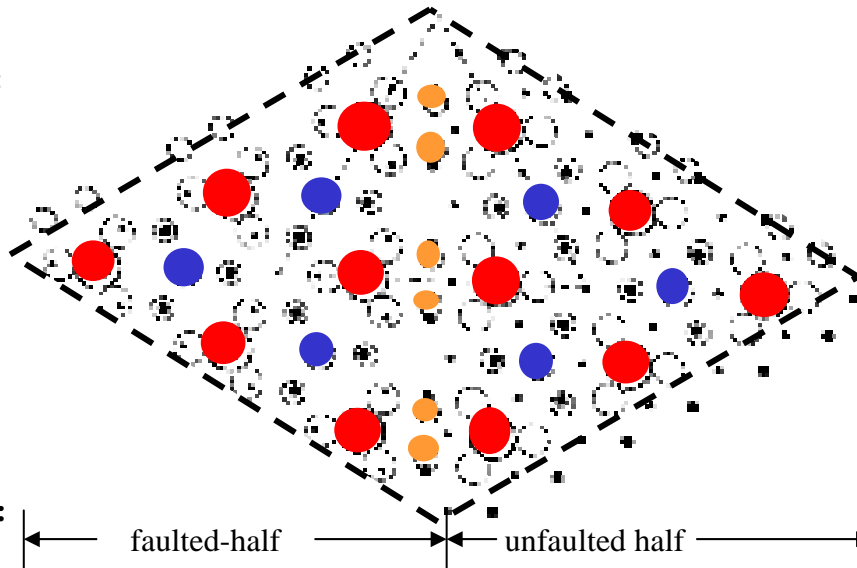
“poly”



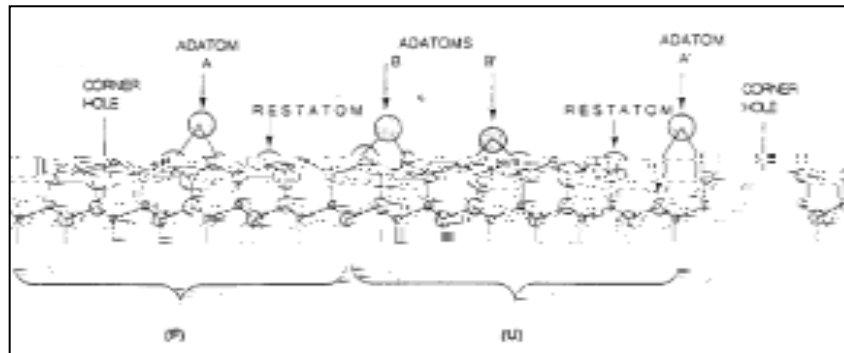


Mapping the Energy Landscape of a Si monomer adsorbed on the reconstructed Si(111)-(7x7) Surface

Top view:

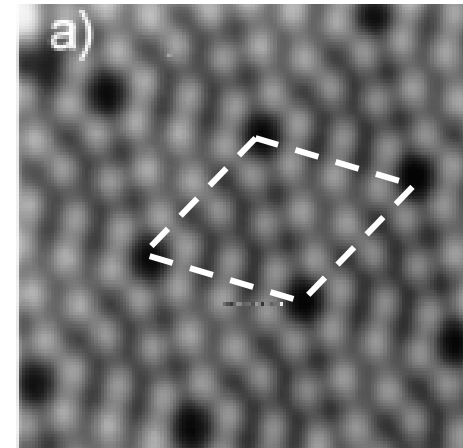


Side view:



- adatoms
- first layer atoms (● rest atoms)
- second layer atoms (● dimers)
- third layer atoms
- fourth layer atoms

STM image of the reconstructed Si(111)-7x7 surface



B. C. Stipe et al. Phys. Rev. Lett. 79, 4397 (1997)

Si(111)-(7x7) dimer-adatom-stacking-fault (DAS)-reconstructed surface: The (7x7) unit cell is indicated by the dashed lines, and the irreducible region is enclosed by the dotted lines.

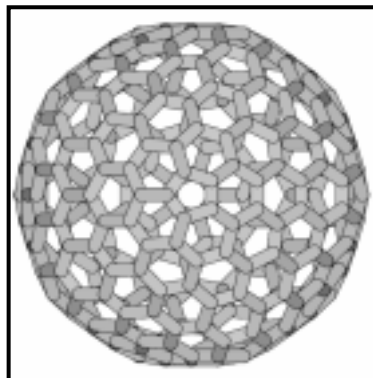
Applications of the SCED/LCAO Hamiltonian

— Predicting structures and properties of silicon/carbon-based nanostructures —

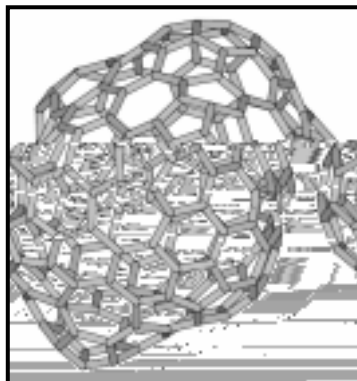
- The totality of carbon clusters
- Silicon Nanowires from a few to ~15 nm
- Silicon carbide clusters
- Silicon carbide nanowires
- Initial stage of growth of carbon single-wall nanotubes

Families of carbon clusters

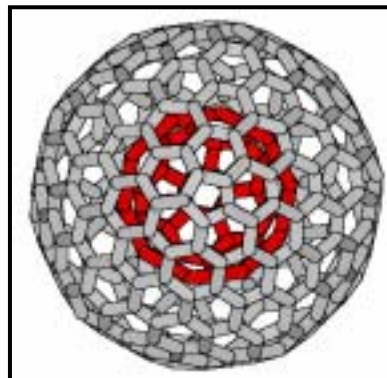
Fullerenes
(sp^2)



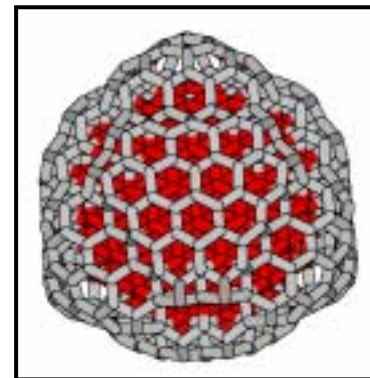
Cages
(sp^2)



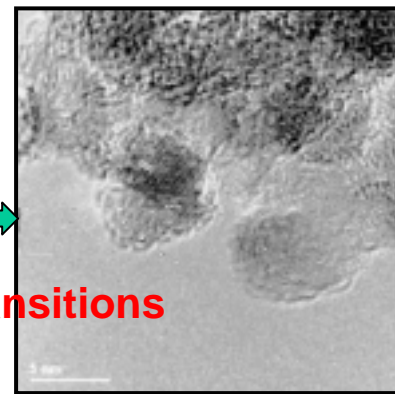
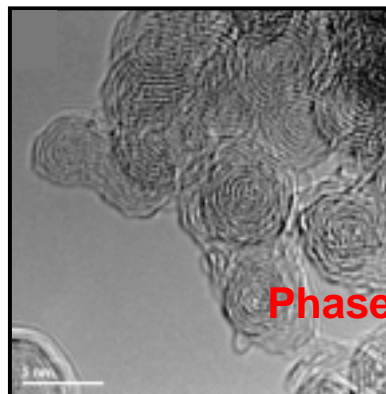
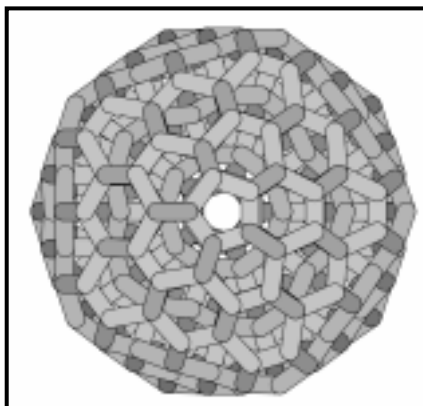
Onions
(sp^2)



bucky-diamonds
(sp^2/sp^3)



Icosahedrons
(sp^2/sp^3)

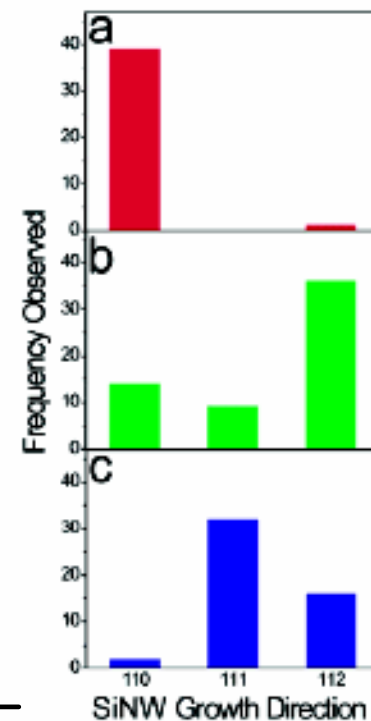
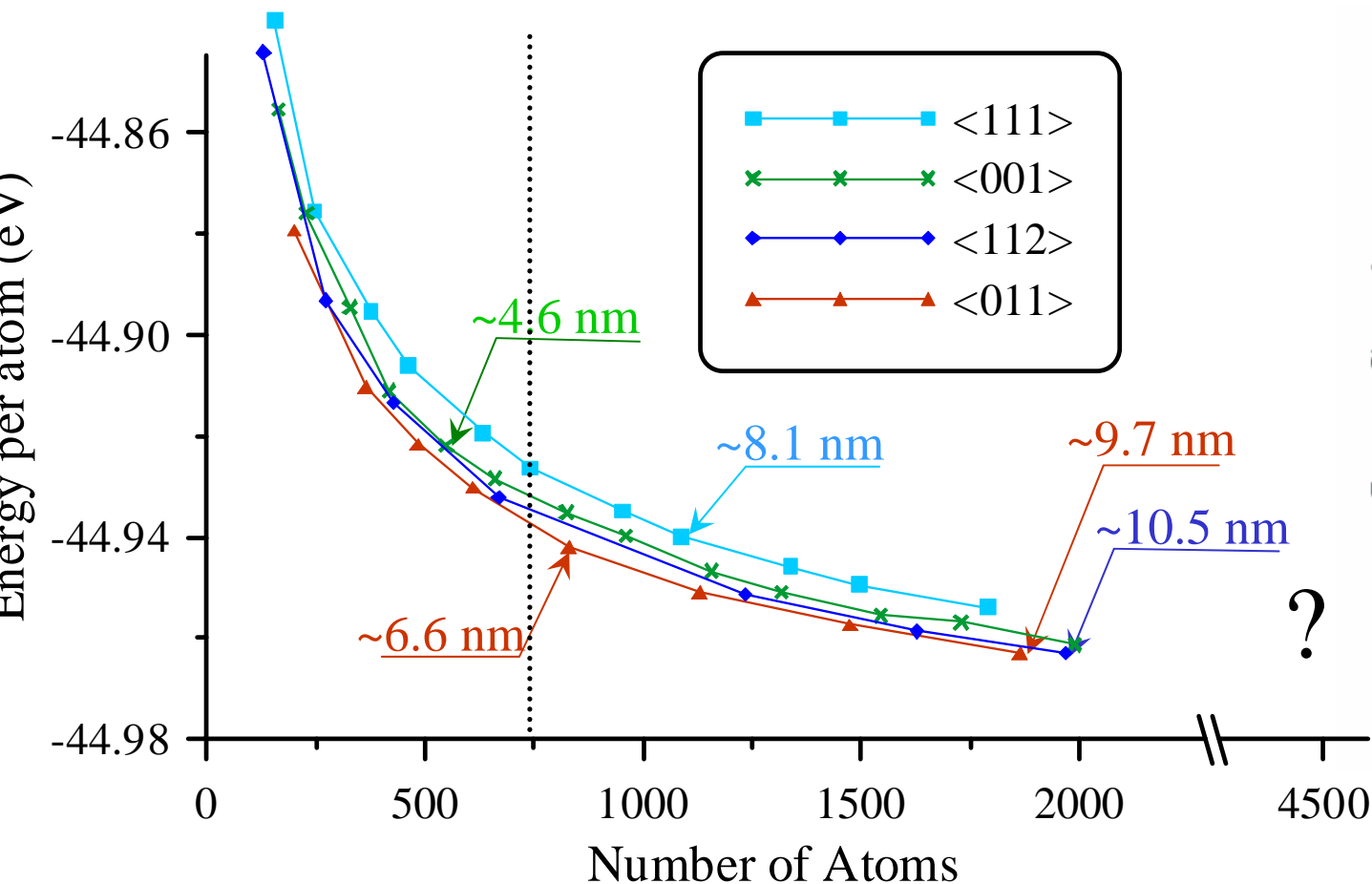


Phase transitions


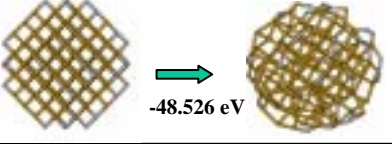

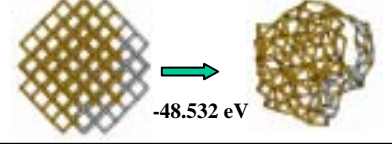
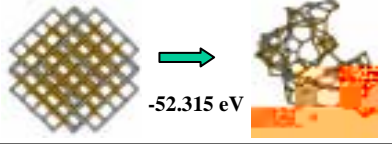


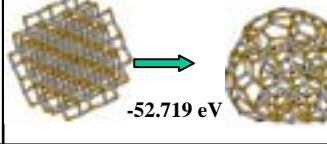
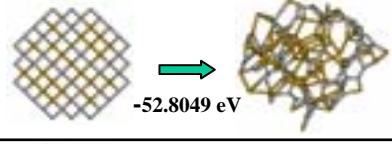


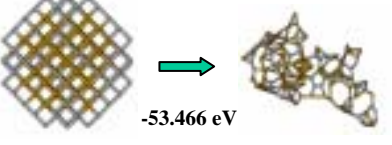

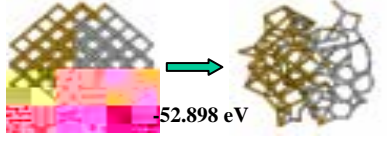
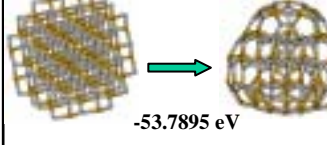
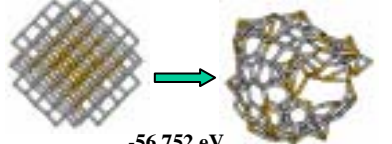
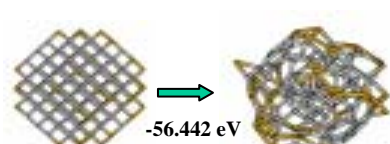

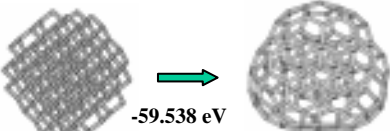
O. O. Myhaylyk et al. J. Appl. Phys. 97, (2005); F. Banhart, J. Appl. Phys. 81, 3440 (1997)

Stability of the nanowires

Wu et al, Nano Lett,
4, 433, (2004)

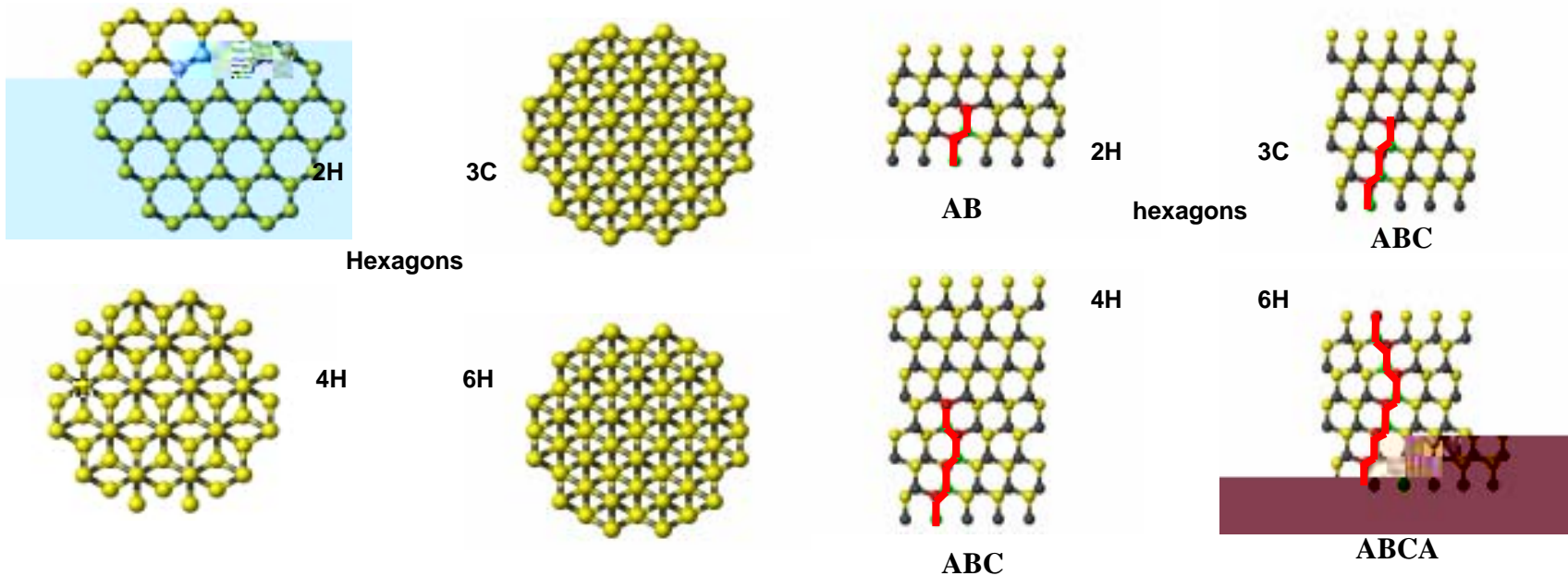


Stabilities of Si_nC_m clusters constructed from a tetrahedral network with various configurations ($n+m=147$)

composition	Si_n -core/ C_m -shell	C_m -core/ Si_n -shell	Segregation	Cut from bulk SiC
Si_{147}				
$\text{Si}_{112}\text{C}_{35}$				
$\text{Si}_{79}\text{C}_{68}$				
$\text{Si}_{73}\text{C}_{74}$				
$\text{Si}_{68}\text{C}_{79}$				
$\text{Si}_{35}\text{C}_{112}$				
C_{147}				

Morphology and stability of SiC NWs

Initial configurations of hexagonal SiC NWs

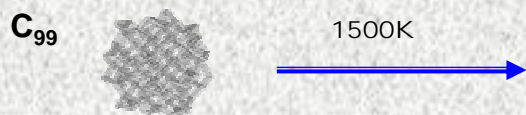
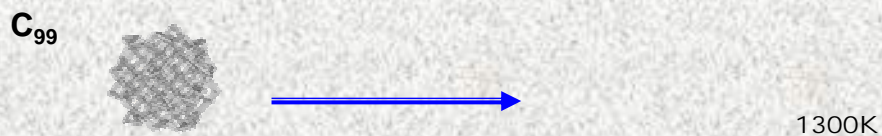
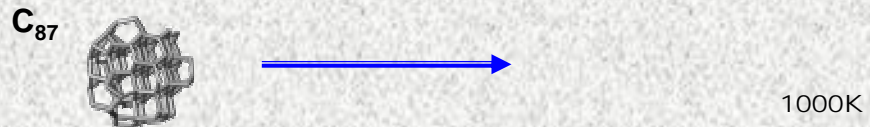


Cross-Sections of SiC NWs

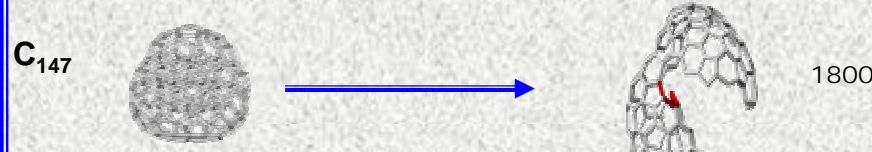
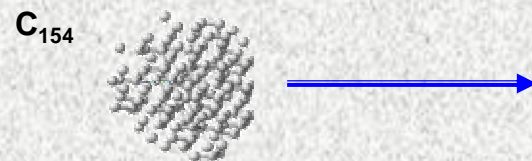
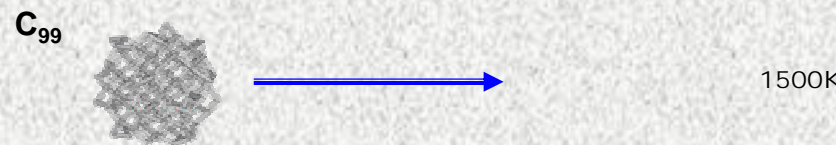
Side-Views of SiC NWs

Results

Jellium medium (Without boundary)



Jellium medium (With boundary)



Relative Stabilities of Silicon Nanowires of Different Orientations

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Department of Physics

University of Louisville

Collaborators: Drs. A. Tchernatinsky, D. Mihas, M. Yu, C.S. Jayanthi

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Motivation

Ø Si Nanowires (SiNW) are a promising material for future electronics applications. FET Transistors (Morales, Lieber, Science **279**, 208 (1998)) and sensors (Cui, et al, Science **293**, 1289 (2001)) have already been demonstrated.

	3-10 nm	10-20 nm	20-30 nm
Y.Wu, et al, Nanolett. 4 ,433 (2004). Vapour-Liquid-Solid.	<011> - 95%, <112>	<112> - 61%, <011>, <111>	<111> - 34%, <112>
I.D.Holms, et al, Science 287 ,1471 (2000). Solution-Phase Synthetic Method.	<011> <001>		
G.W.Zhou, et al, APL 73 , 677 (1998). Las. Abl.		<112>	
X. Lu et al, Nanolett. 3 , 93 (2003). Supercritical Fluid-Liquid-Solid.	<011>		
S. Ge et al, Adv. Mater. 17 , 56 (2005). VLS.			<111>

Ø There are theoretical works on the electronic structure of SiNWs (Zhao, et al, PRL, 92, 236805, (2004) and ref. therein). Structure and morphology – limited (PRB, **57**, 11923 and PRL, **94**, 026208).

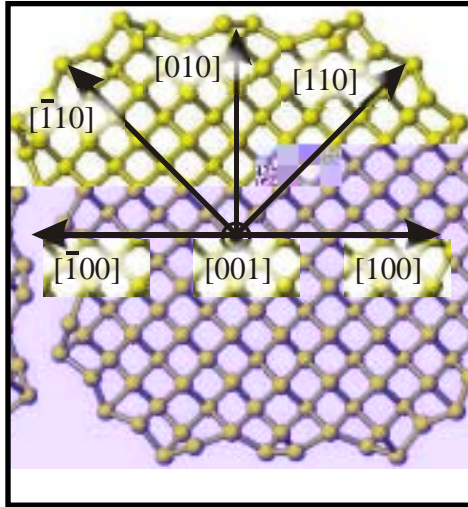
Ø In this work we are presenting the results of a comprehensive study of the morphology and stability of SiNWs along directions reported in the experimental papers. Calculations are performed in *ab initio* (VASP) and tight-binding (SCED-LCAO) frameworks.

Computational procedure

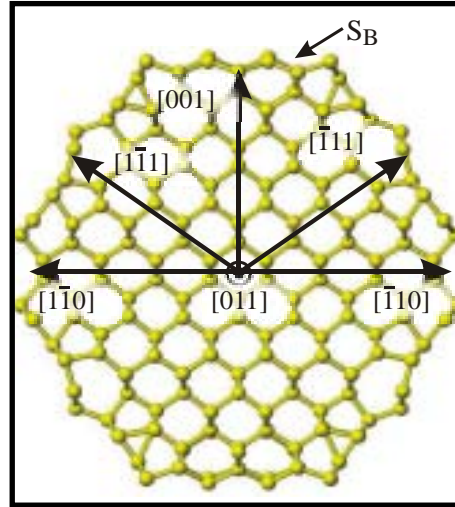
- Ø Determine the most favorable surface reconstructions and shape for small size SiNWs in the $\langle 001 \rangle$, $\langle 011 \rangle$, $\langle 111 \rangle$, and $\langle 112 \rangle$ directions using *ab initio* calculations (we consider non-passivated SiNWs in order to be able to compare total energies).
- Ø The only requirement for the reconstruction – no surface atoms with more than one dangling bond.
- Ø Hydrogen or oxide passivation, kinetic effects (exp. $T \sim 500^\circ \text{C}$), effects of gold-silicon interface (for the VLS growth) and such are not taken into account.
- Ø VASP parameters: GGA (PW91), $E_{\text{cutoff}} = 200 \text{ eV}$, k-point mesh ($1 \times 1 \times 10$) for the smaller, and ($1 \times 1 \times 6$) for larger (> 500 atoms in the system).
- Ø Repeat these calculations in the SCED-LCAO framework, making sure that transferability of the parameters is not a problem.
- Ø Expand the size of the system to the 10 nm level and beyond utilizing ‘Order-N’ method on top of the SCED-LCAO semi-empirical Hamiltonian.

Relaxed Structures of SiNWs oriented along different directions

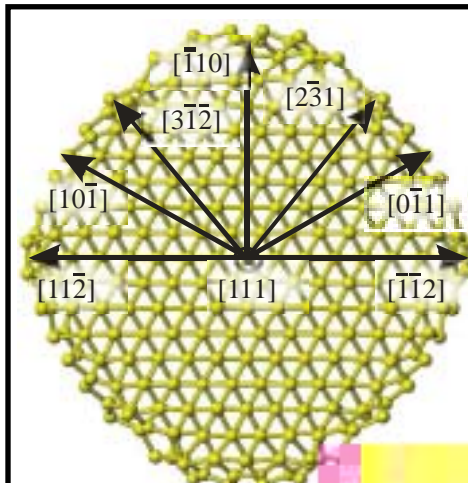
$\langle 001 \rangle$



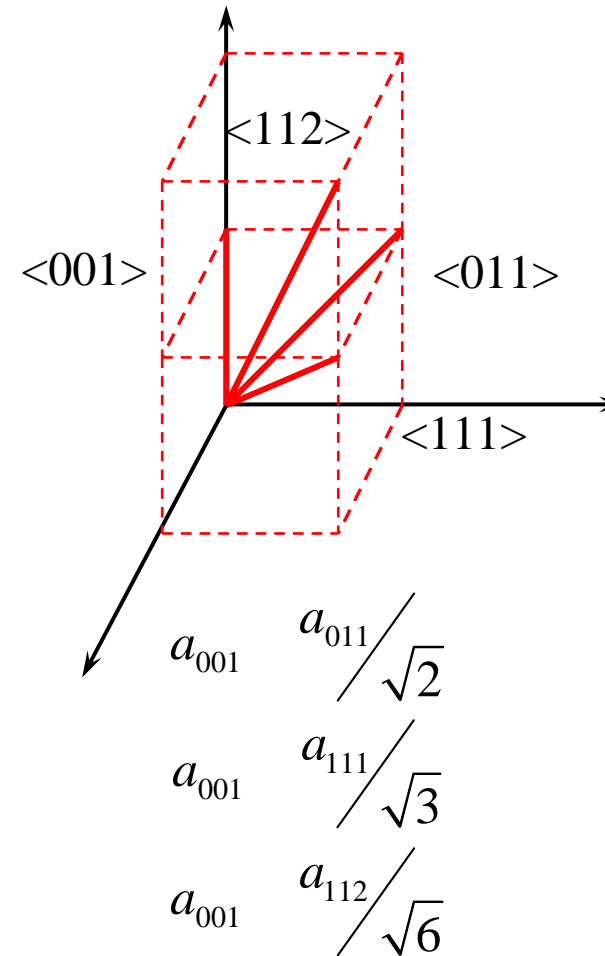
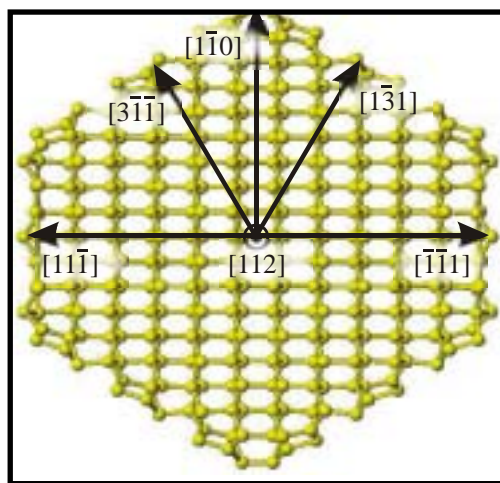
$\langle 011 \rangle$



$\langle 111 \rangle$

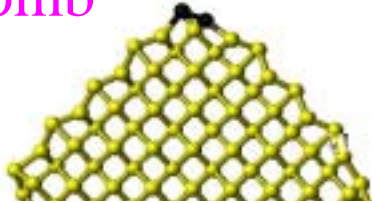


$\langle 112 \rangle$

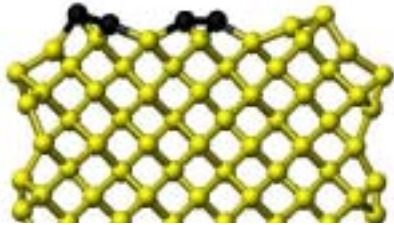


Morphology of $\langle 001 \rangle$ nanowires

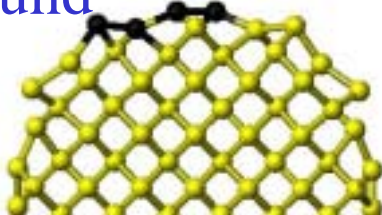
“rhomb”



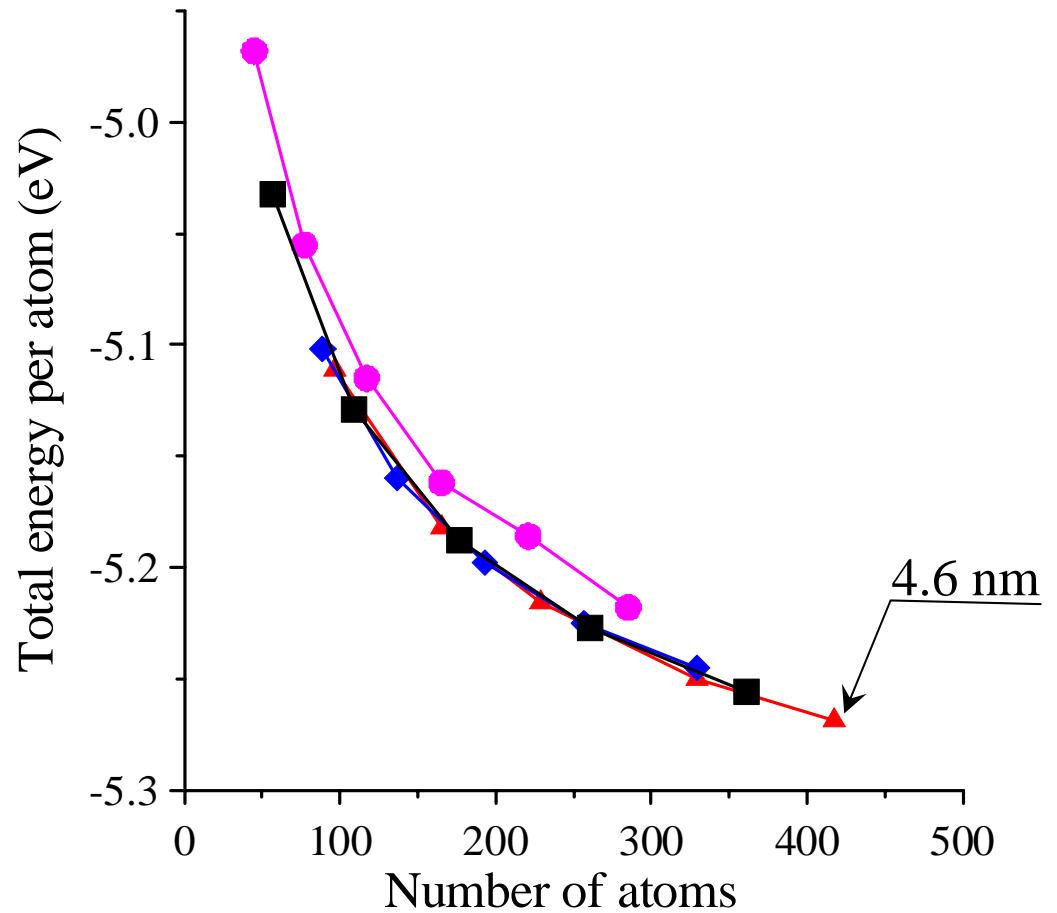
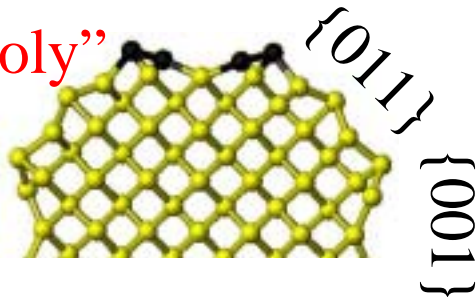
“square”



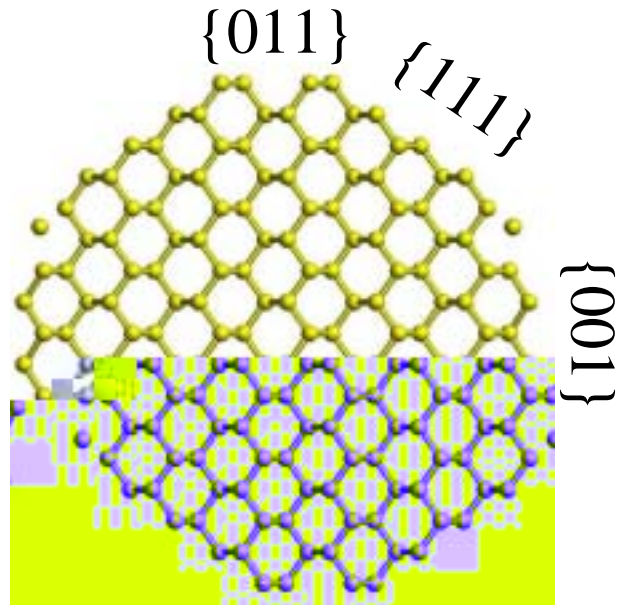
“round”



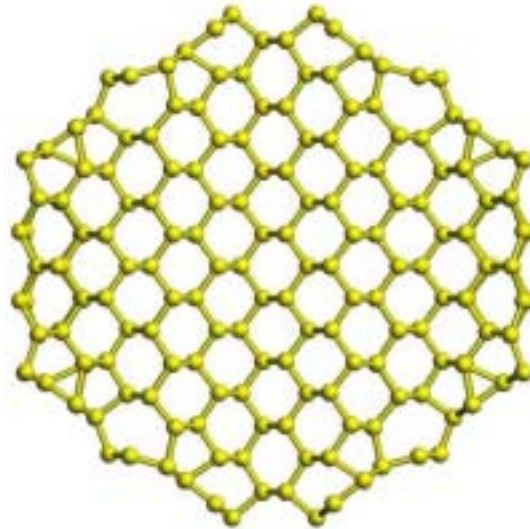
“poly”



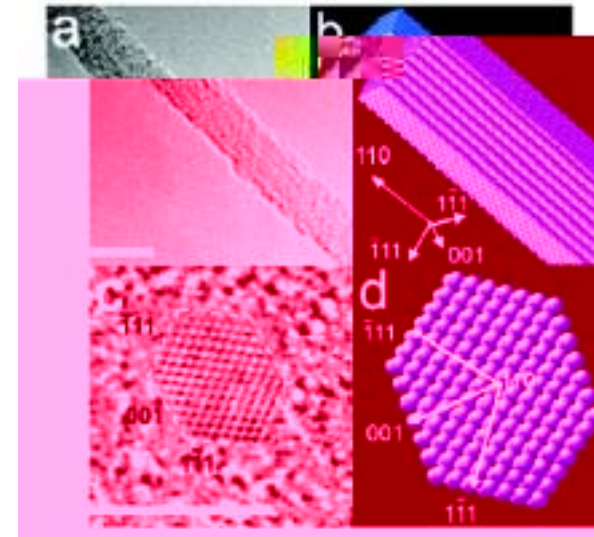
Morphology of $\langle 011 \rangle$ nanowires



As cut



Relaxed

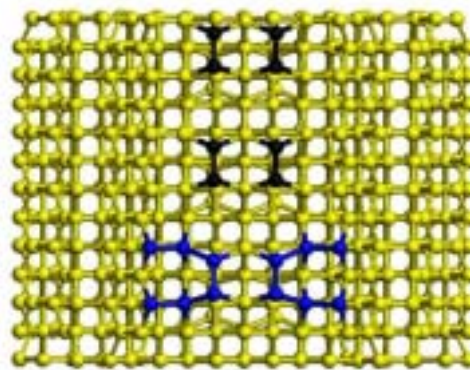


Experiment

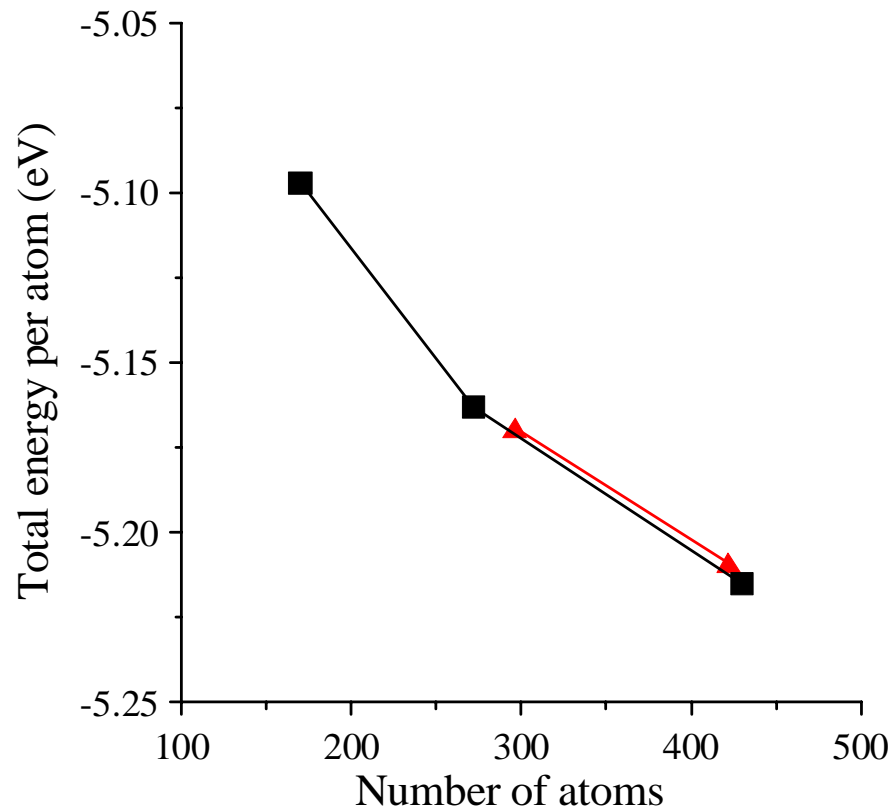
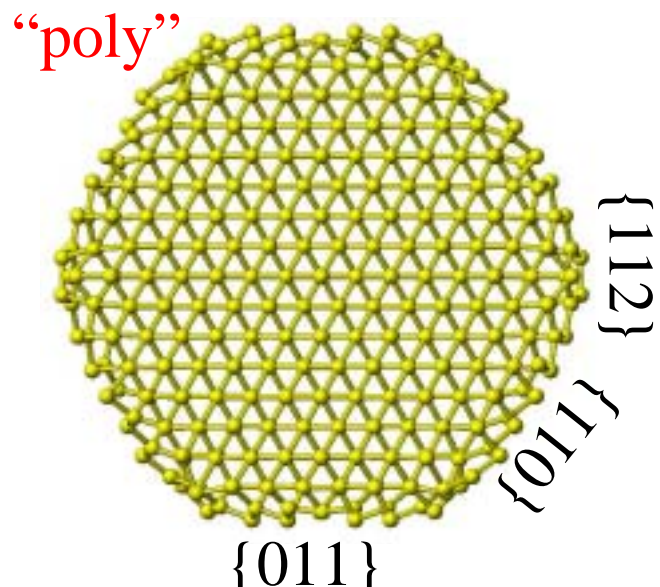
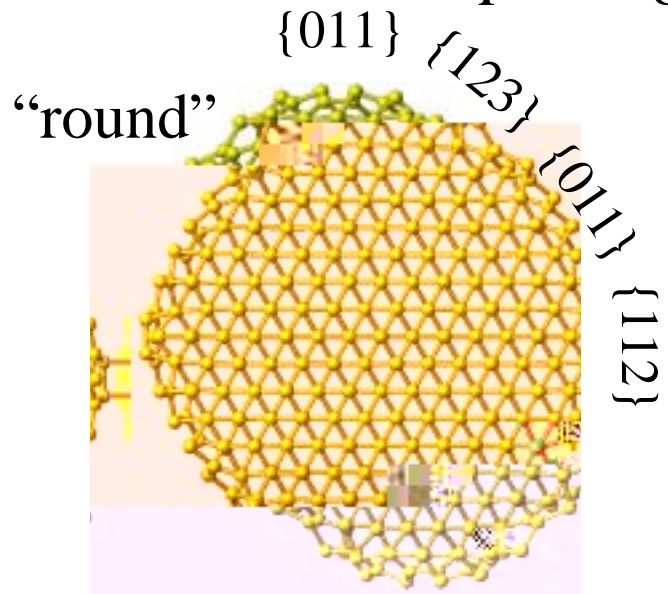
(Wu et al, Nano Lett, **4**, 433, 2004)

Lateral view:

Illustration of the S_B step

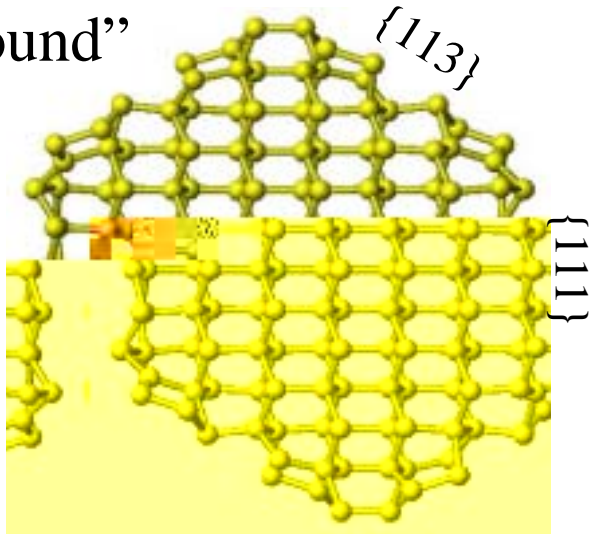


Morphology of $\langle 111 \rangle$ nanowires

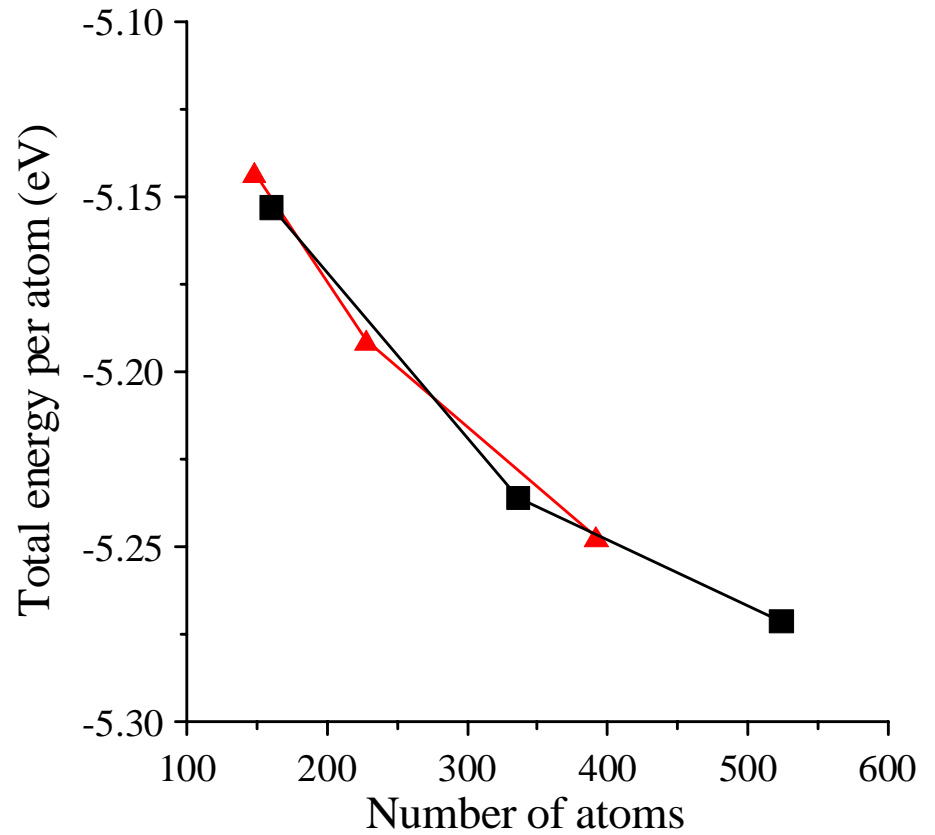
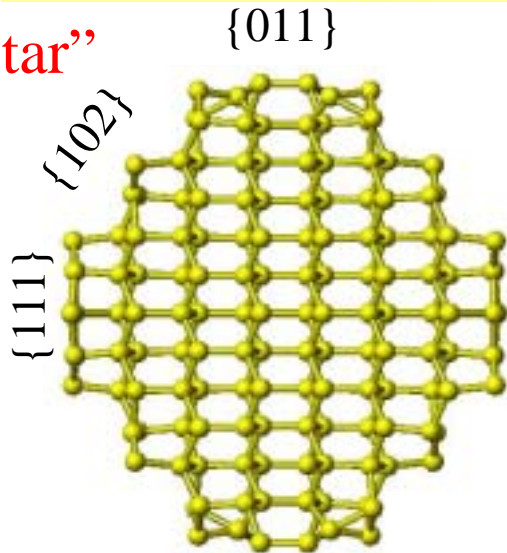


Morphology of $\langle 112 \rangle$ nanowires

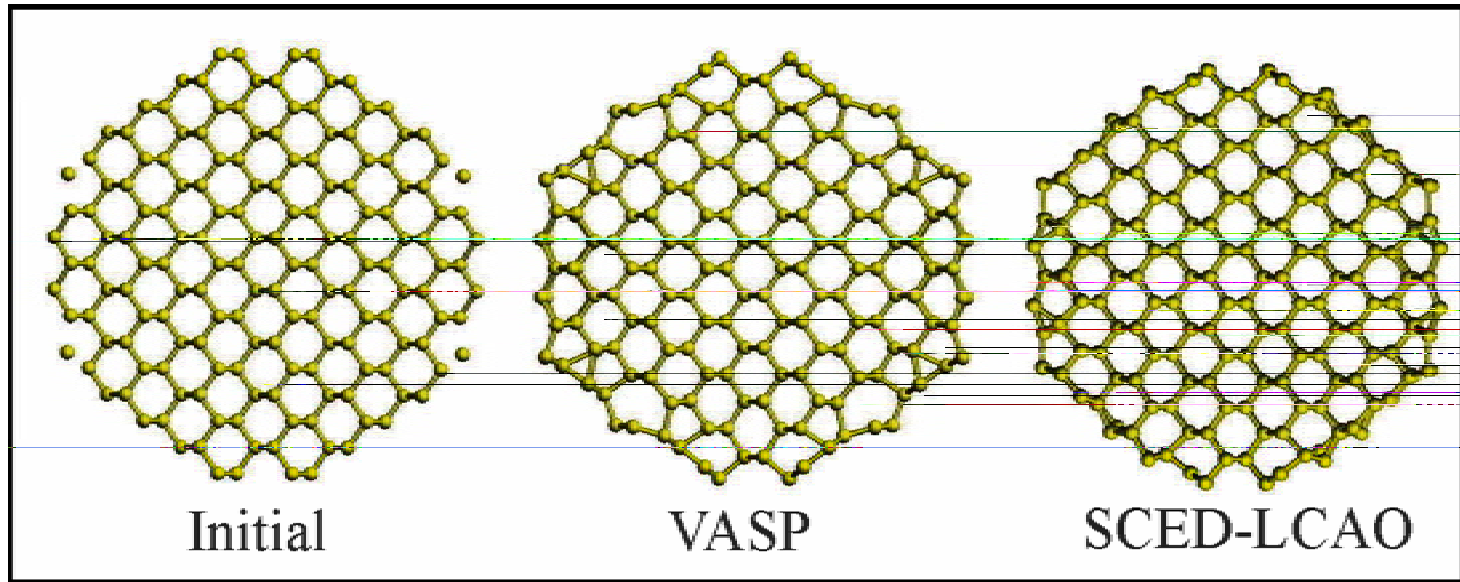
“round”



“star”



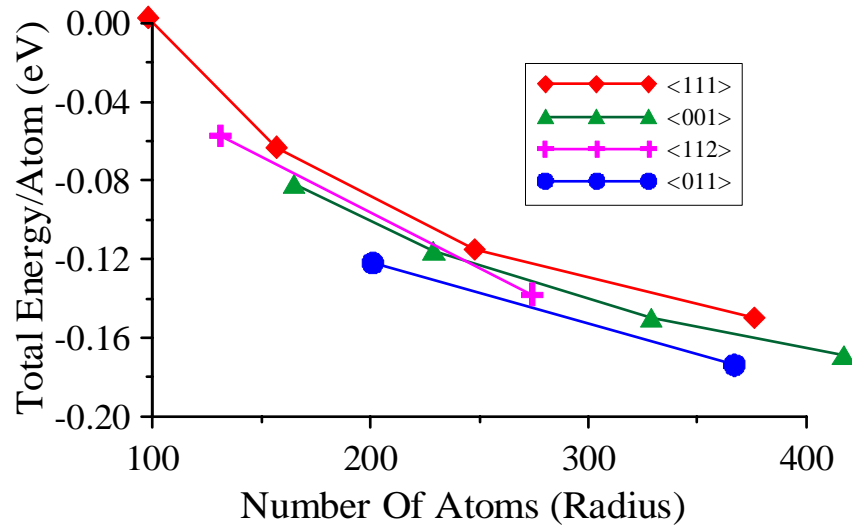
Surface Morphologies



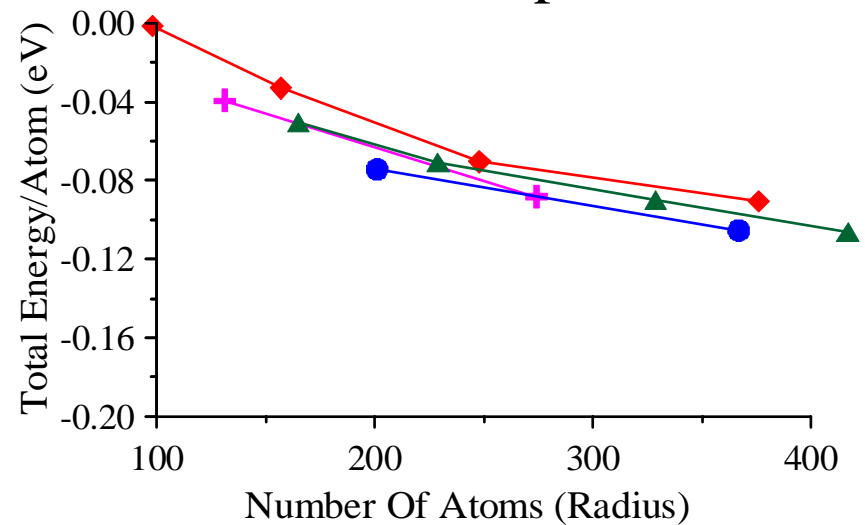
A comparison of the structures obtained by ab-initio and SCED-LCAO methods for SiNWs oriented in $\langle 011 \rangle$ direction ($d \sim 4.7$ nm)

Comparison of the USPP and SCED-LCAO results

Ab-initio



Semi-empirical

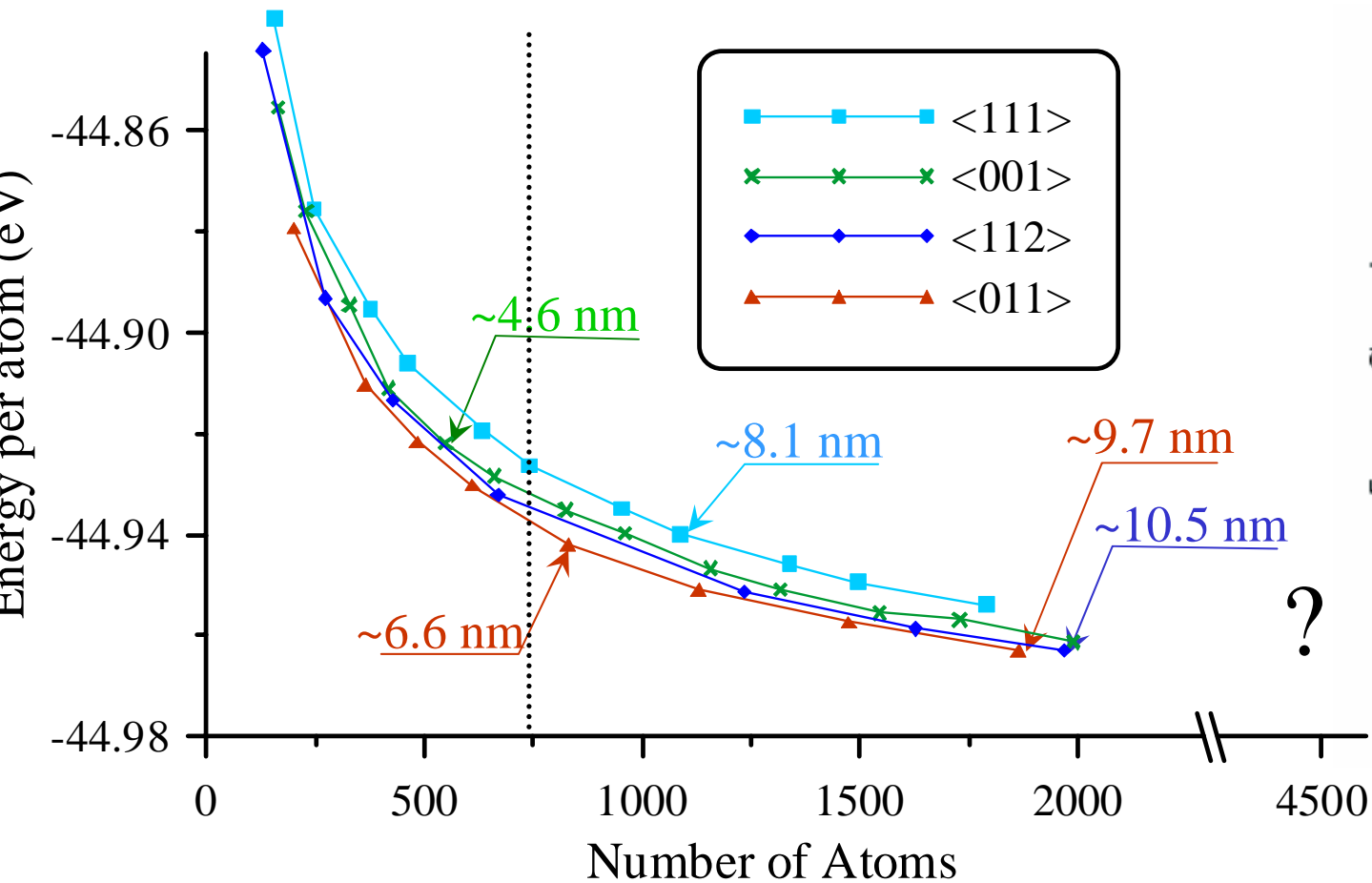


Ø Great qualitative agreement between two methods.

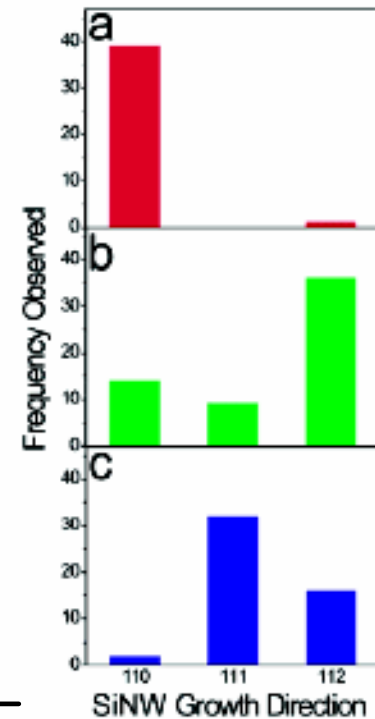
Ø The energetic ordering of the nanowires along the same direction but different morphologies is also correct in SCED-LCAO.

Ø Equilibrium lattice parameter for SCED-LCAO is always within 2% of the *ab initio* calculations.

Stability of the nanowires



Wu et al, Nano Lett,
4, 433, (2004)



Conclusions

Ø Most energetically favored morphologies of the small (up to 3 nm) non-passivated SiNWs are determined through first-principles calculations for 4 different directions of growth.

Ø Very good agreement in the ordering of the energies of the different orientations and morphologies between first-principles and SCED-LCAO tight-binding approaches.

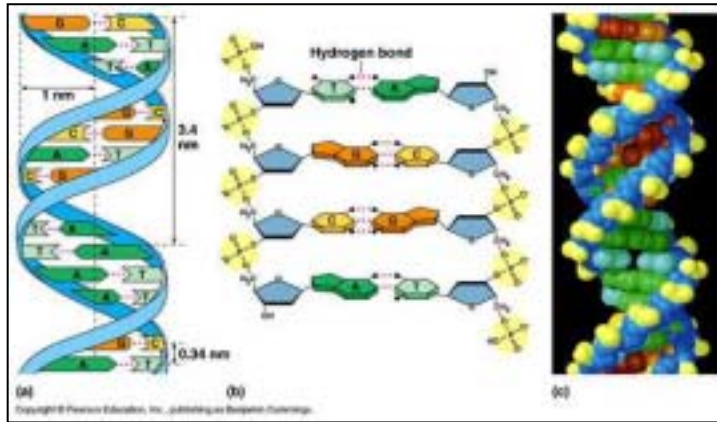
Ø In the < 10 nm range of the nanowire sizes we predict $<011>$ direction of growth to be thermodynamically most favorable, in agreement with the experimental data.

Ø Future application: Extend the size of the nanowires into ~ 20 nm scale.

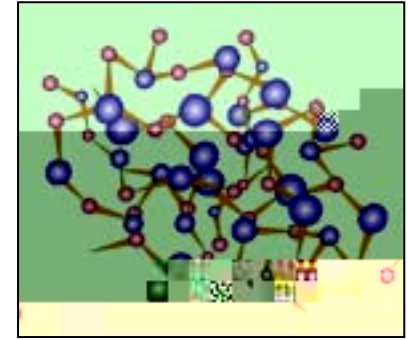
Ø In the SCED-LCAO framework include hydrogen passivation in order to obtain electronic structure information.

Applications for the study of biological and “soft mater” systems

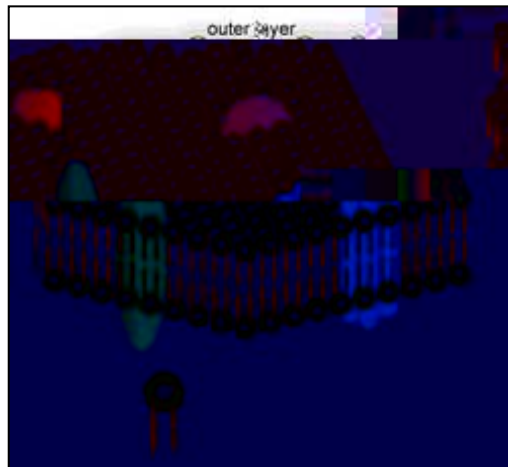
DNA



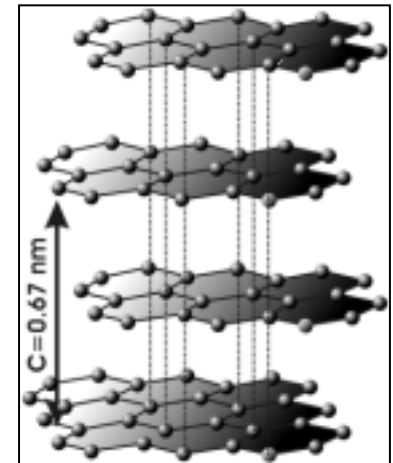
Polymer



Membrane



Graphite



Parallel Replica Dynamics (PRD) and SCED/LCAO-PRD:

A scheme to extend the accessible
Simulation time for quantum
mechanics-based molecular
dynamics simulations

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