

# Simulação Computacional dos Materiais

---

***Caetano Rodrigues Miranda***

***Dra. Elizane Moraes***

***Dra. Michele Salvador***

***AULA 19 – 22/10/2020***

***IFUSP***

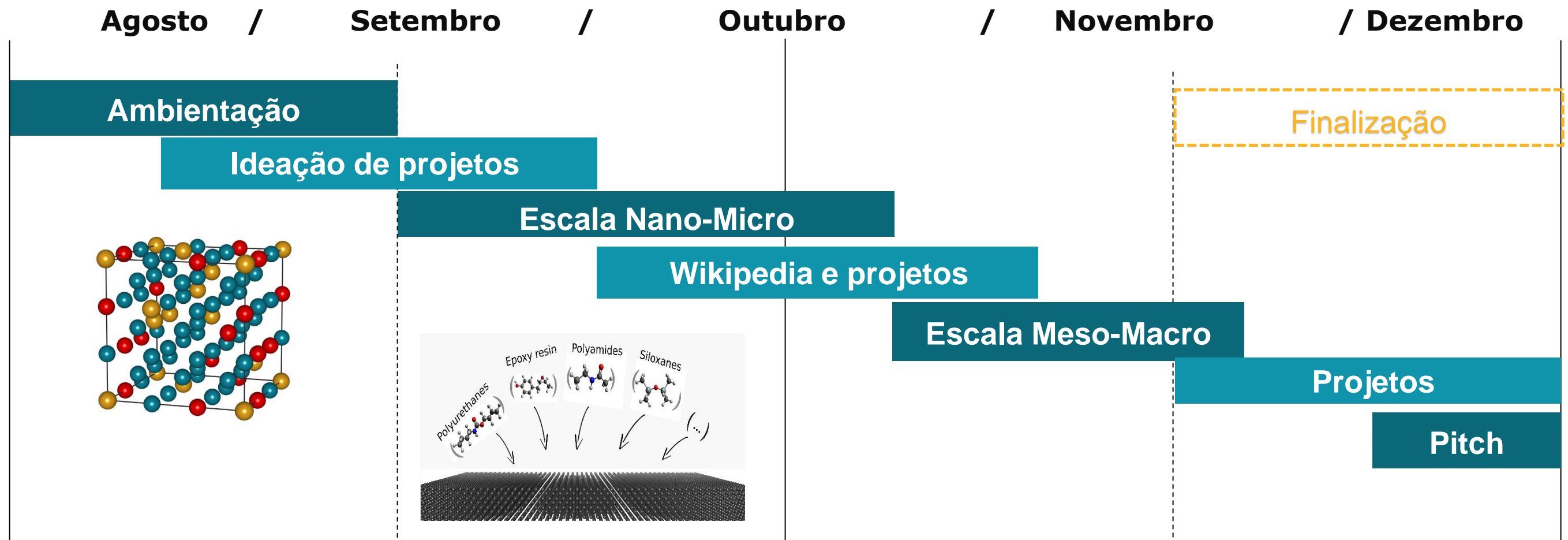
*crmiranda@usp.br*



*sampa*



# Cronograma



**Métodos Multiescala  
Aprendizado de máquina**

# Cronograma

---

DECRETO N° 65.257, DE 19 DE OUTUBRO DE 2020 – alteração de data do feriado pela comemoração do Dia do Funcionário Público do dia 28 para dia 30 de Outubro

29/10 – Colóquio (17:00)

29/10 – Atividade wikipedia

30/10 – Não haverá aula

30/10 – novo prazo para o relatório do lab 4

05/11 – Discussão projetos

06/11 – Aprendizado de Máquina

14/11 – prazo para o relatório lab6

# Wikipedia

---

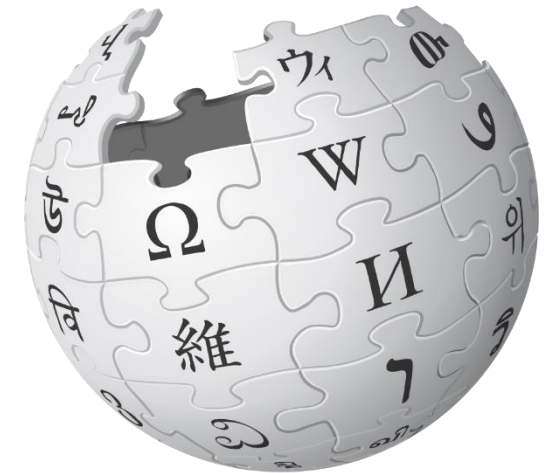
Dinâmica Molecular

Monte Carlo

Cálculos de primeiros princípios

Elementos Finitos

Redes de Boltzmann



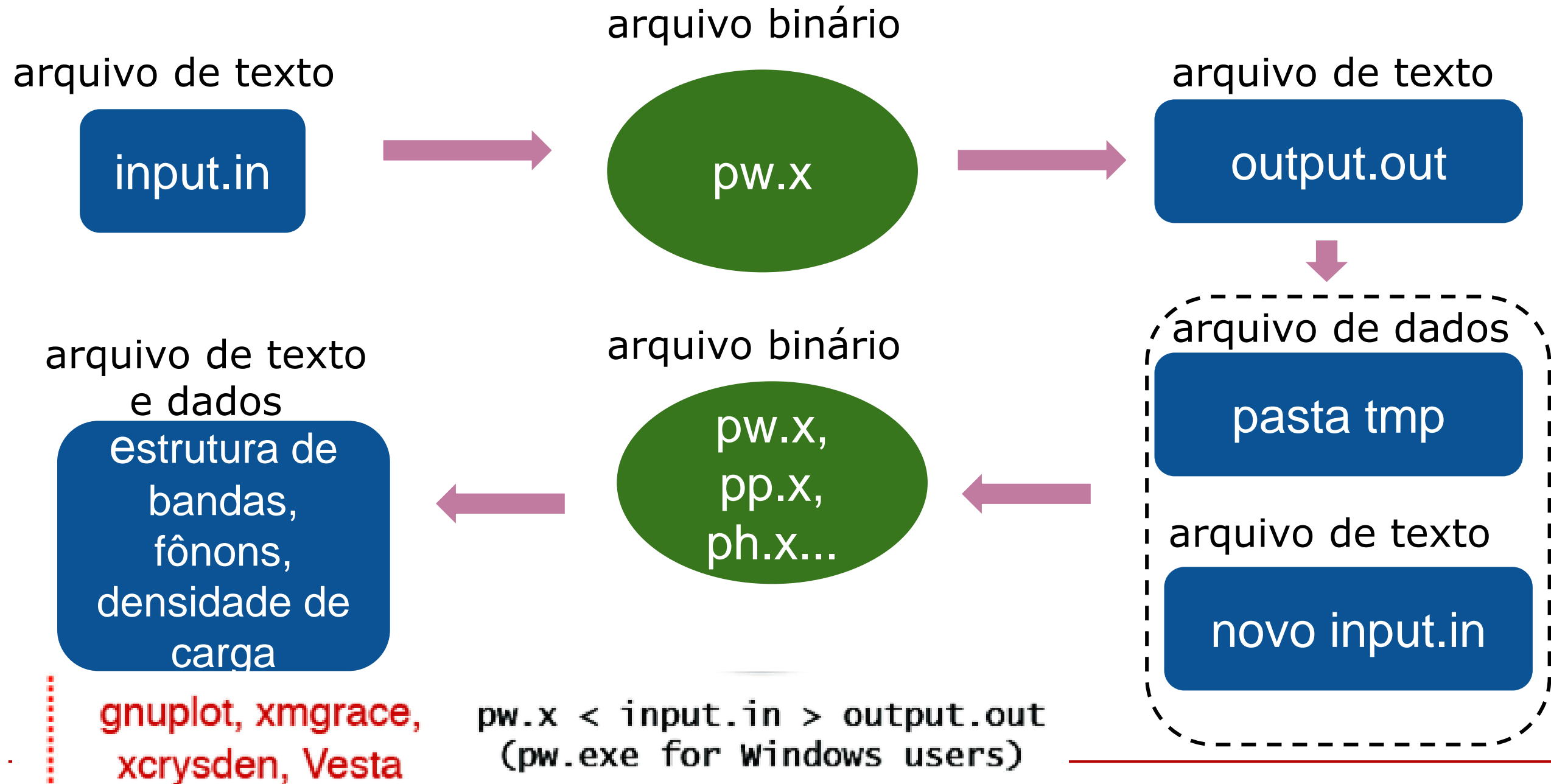
**WIKIPÉDIA**  
A enciclopédia livre



**LABORATÓRIO**  
**CÁLCULOS DE PRIMEIROS PRINCÍPIOS**  
**TEORIA DO FUNCIONAL DA DENSIDADE (DFT)**

---

# Preparação para a prática



# Práticas

---

**Prática 0:** cálculo de relaxação de uma molécula isolada.

Será feito o cálculo de relaxação de uma molécula de metanol em uma caixa. O cálculo de moléculas isoladas é o mais simples e o resultado será utilizado na prática 3.

**Prática 1:** Testes iniciais com o Silício Si; (github)

**Prática 2:** Testes com o Alumínio; (github)

**Prática 3:** Homodímeros de Metanol; (github)

# Resultados Si ...

## Numerical atomic orbitals for linear-scaling calculations

Javier Junquera,<sup>1</sup> Óscar Paz,<sup>1</sup> Daniel Sánchez-Portal,<sup>2,3</sup> and Emilio Artacho<sup>4</sup>

PHYSICAL REVIEW B **64** 235111

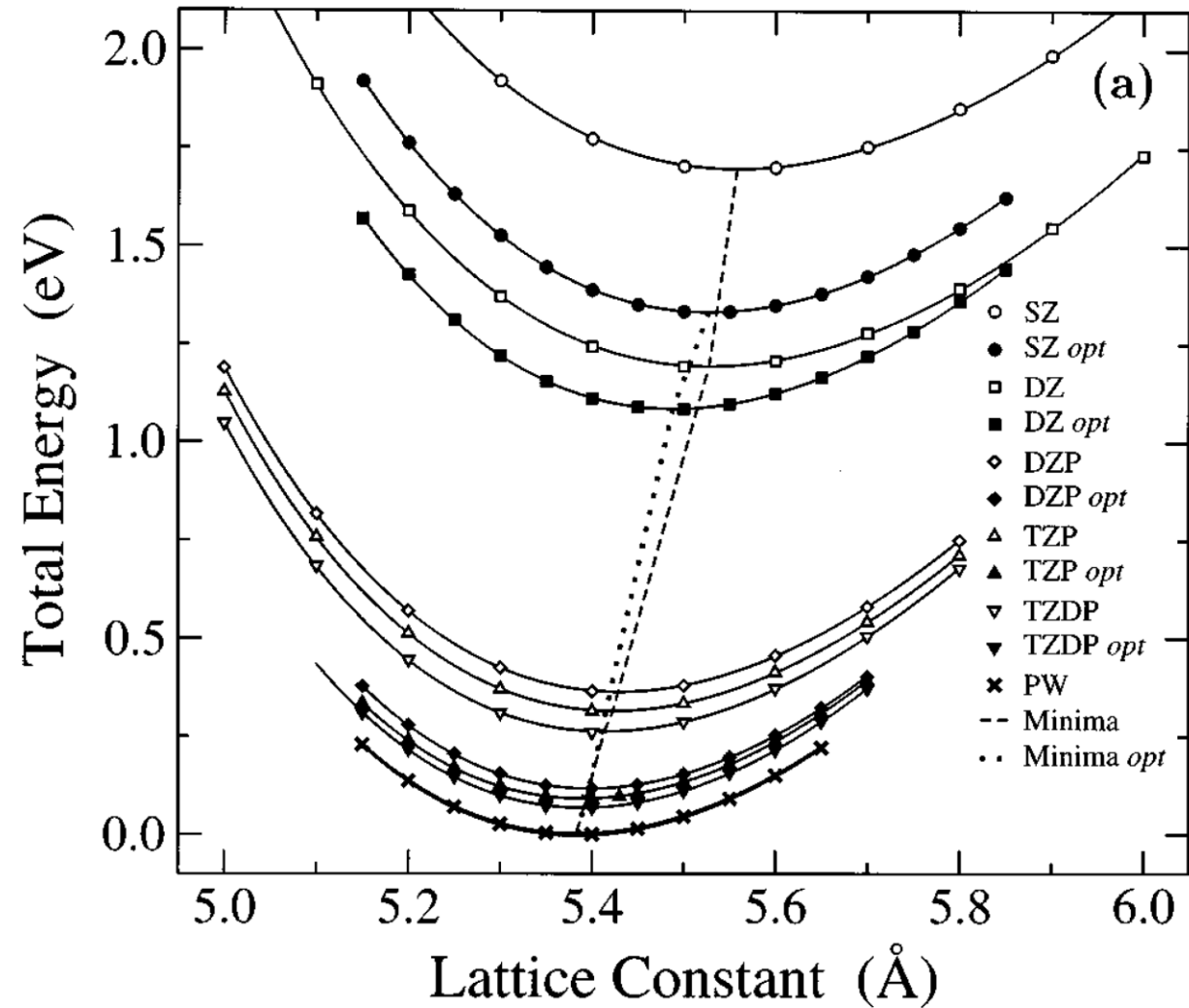


TABLE IV. Basis comparisons for different solids.  $a$ ,  $B$ , and  $E_c$  stand for lattice parameter (in Å), bulk modulus (in GPa), and cohesive energy (in eV), respectively.

		Exp	LAPW	Other PW	PW	DZP
Au	$a$	4.08 <sup>a</sup>	4.05 <sup>b</sup>	4.07 <sup>c</sup>	4.05	4.07
	$B$	173 <sup>a</sup>	198 <sup>b</sup>	190 <sup>c</sup>	191	188
	$E_c$	3.81 <sup>a</sup>	-	-	4.19	4.03
MgO	$a$	4.21 <sup>d</sup>	4.26 <sup>e</sup>	-	4.10	4.11
	$B$	152 <sup>d</sup>	147 <sup>e</sup>	-	168	167
	$E_c$	10.30 <sup>d</sup>	10.40 <sup>e</sup>	-	11.90	11.87
C	$a$	3.57 <sup>a</sup>	3.54 <sup>f</sup>	3.54 <sup>g</sup>	3.53	3.54
	$B$	442 <sup>a</sup>	470 <sup>f</sup>	436 <sup>g</sup>	466	453
	$E_c$	7.37 <sup>a</sup>	10.13 <sup>f</sup>	8.96 <sup>g</sup>	8.90	8.81
Si	$a$	5.43 <sup>a</sup>	5.41 <sup>h</sup>	5.38 <sup>g</sup>	5.38	5.40
	$B$	99 <sup>a</sup>	96 <sup>h</sup>	94 <sup>g</sup>	96	97
	$E_c$	4.63 <sup>a</sup>	5.28 <sup>h</sup>	5.34 <sup>g</sup>	5.37	5.31



# Novas formas de estruturas cristalinas ...

VOLUME 67, NUMBER 6

PHYSICAL REVIEW LETTERS

5 AUGUST 1991

## New Low-Energy Crystal Structure for Silicon

L. L. Boyer, Efthimios Kaxiras,<sup>(a)</sup> J. L. Feldman, J. Q. Broughton, and M. J. Mehl  
*Complex Systems Theory Branch, Naval Research Laboratory, Washington, D.C. 20375-5000*  
(Received 28 February 1991)

A minimum-energy path in strain space has been determined which takes cubic silicon into itself. Energies are computed using the Stillinger-Weber model potential and first-principles total-energy calculations. The energy along this path has an additional minimum, corresponding to a crystal structure with a body-centered-tetragonal lattice and fivefold-coordinated atoms. Lattice-dynamics, molecular-dynamics, and elastic-constant calculations show the structure is stable.

PACS numbers: 61.55.Dc, 61.42.+h, 64.70.Kb, 71.25.Rk

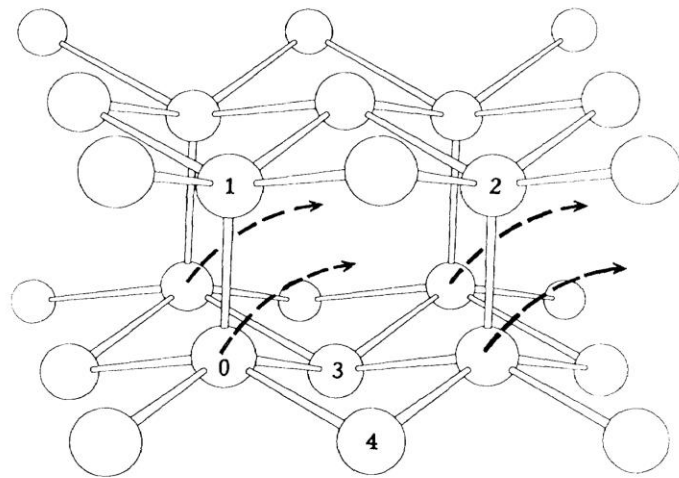


FIG. 2. The bct5 structure with structural parameters as indicated. Two sixfold rings lying in perpendicular (110) planes are denoted by solid and dashed bonds.

Having demonstrated the stability of the bct5 structure, we now consider the prospects for making it experimentally. The magic-strain path (Fig. 1) starts out primarily as a contraction along the (0.3347, 0.8991, 0.2822) direction relative to the usual axes of a cubic crystal. Thus, we propose applying uniaxial stress along this special direction. Since the magic-strain path is a minimum-energy path, the remaining structural parameters should, in principle, follow approximately that predicted in Fig. 1. The difficulty will likely be in preventing fracture before reaching the bct5 structure. Thus, a sudden application of stress, as in a shock experiment, may be preferable. Hydrostatic pressure, in combination with uniaxial stress, might help produce the desired transformation and prevent fracture.

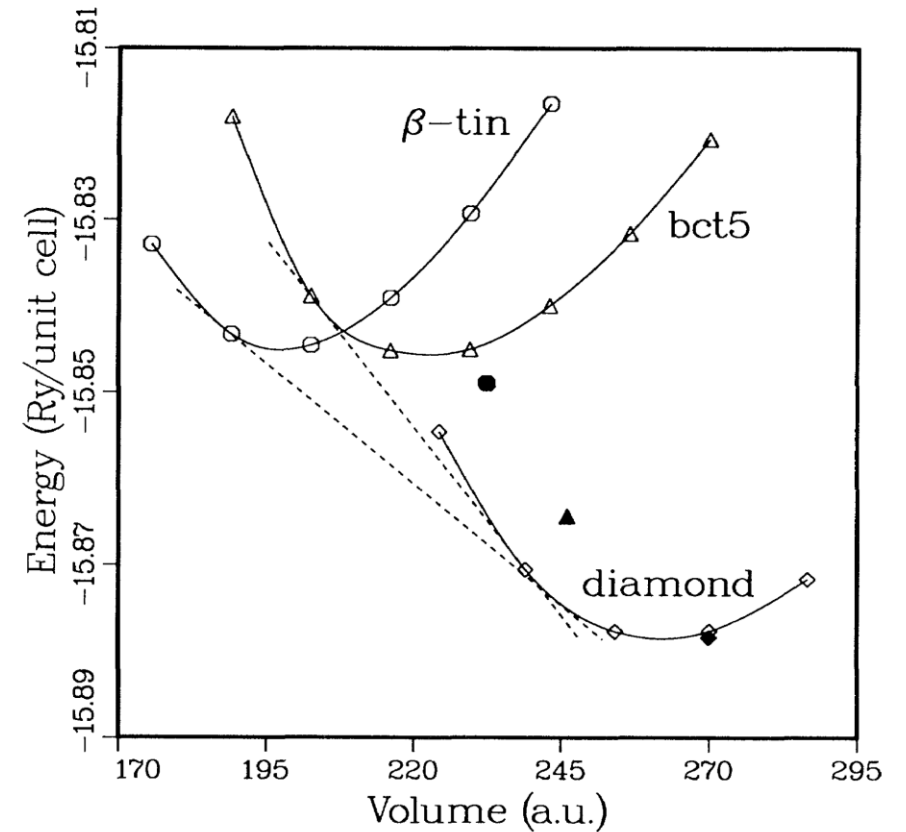


FIG. 3. Energy as a function of volume for the  $\beta$ -Sn ( $\circ$ ), bct5 ( $\triangle$ ), and diamond ( $\diamond$ ) structures. Solid lines are fitted to results of PS calculations (open symbols). Solid symbols are SW results for minimum energy and corresponding volume, with the energy scale shifted to match that of the PS diamond structure. Slopes of the dashed lines give transition pressures for cubic to  $\beta$ -Sn (84 kbar) and cubic to bct5 (126 kbar).

# Comparação com a literature ...

## Fit parameters:

$$V_0 = 39.4633 \text{ \AA}^3$$

$$E_0 = -216.3188 \text{ eV}$$

$$B(V_0) = 0.5768 \text{ eV/\AA}^3$$

$$B'(V_0) = 4.1989$$

**Theoretical lattice parameter: 5.4044 \AA**

**92,41 GPa**

**(1 eV / \AA<sup>3</sup> = 160,2176487 GPa)**

TABLE IV. Basis comparisons for different solids.  $a$ ,  $B$ , and  $E_c$  stand for lattice parameter (in \AA), bulk modulus (in GPa), and cohesive energy (in eV), respectively.

		Exp	LAPW	Other PW	PW	DZP
Au	$a$	4.08 <sup>a</sup>	4.05 <sup>b</sup>	4.07 <sup>c</sup>	4.05	4.07
	$B$	173 <sup>a</sup>	198 <sup>b</sup>	190 <sup>c</sup>	191	188
	$E_c$	3.81 <sup>a</sup>	-	-	4.19	4.03
MgO	$a$	4.21 <sup>d</sup>	4.26 <sup>e</sup>	-	4.10	4.11
	$B$	152 <sup>d</sup>	147 <sup>e</sup>	-	168	167
	$E_c$	10.30 <sup>d</sup>	10.40 <sup>e</sup>	-	11.90	11.87
C	$a$	3.57 <sup>a</sup>	3.54 <sup>f</sup>	3.54 <sup>g</sup>	3.53	3.54
	$B$	442 <sup>a</sup>	470 <sup>f</sup>	436 <sup>g</sup>	466	453
	$E_c$	7.37 <sup>a</sup>	10.13 <sup>f</sup>	8.96 <sup>g</sup>	8.90	8.81
Si	$a$	5.43 <sup>a</sup>	5.41 <sup>h</sup>	5.38 <sup>g</sup>	5.38	5.40
	$B$	99 <sup>a</sup>	96 <sup>h</sup>	94 <sup>g</sup>	96	97
	$E_c$	4.63 <sup>a</sup>	5.28 <sup>h</sup>	5.34 <sup>g</sup>	5.37	5.31

$$E(V) = E_0 + \frac{9V_0 B_0}{16} \left\{ \left[ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right]^3 B'_0 + \left[ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right]^2 \left[ 6 - 4 \left( \frac{V_0}{V} \right)^{\frac{2}{3}} \right] \right\}.$$

# Novos materiais ...

THE JOURNAL OF CHEMICAL PHYSICS 137, 034703 (2012)

## Comparison of thermodynamic stabilities and mechanical properties of CO<sub>2</sub>, SiO<sub>2</sub>, and GeO<sub>2</sub> polymorphs by first-principles calculations

Mia Ledyastuti,<sup>1</sup> Yunfeng Liang,<sup>1,a)</sup> Caetano R. Miranda,<sup>1,2,a)</sup> and Toshifumi Matsuoka<sup>1,a)</sup>

<sup>1</sup>Environment and Resource System Engineering, Kyoto University, Kyoto 615-8540, Japan

<sup>2</sup>Universidade Federal do ABC, Rua Santa Adélia, 166 Bangu 09210-170, Santo André, SP Brazil

(Received 27 April 2012; accepted 21 June 2012; published online 18 July 2012)

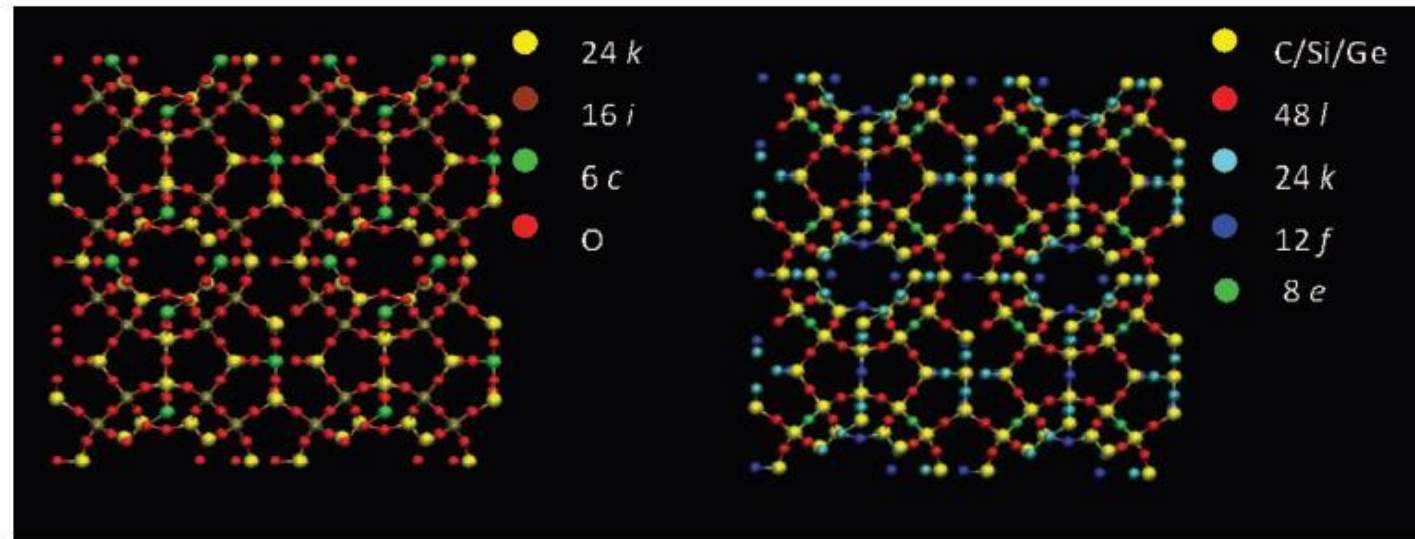


FIG. 1. Crystal structure of CO<sub>2</sub>, SiO<sub>2</sub> and GeO<sub>2</sub> clathrate. Carbon, silicon, and germanium were classified into three sites (24*k*, 16*i* and 6*c*); meanwhile, oxygen was classified into four sites (48*l*, 24*k*, 12*f*, and 8*e*).

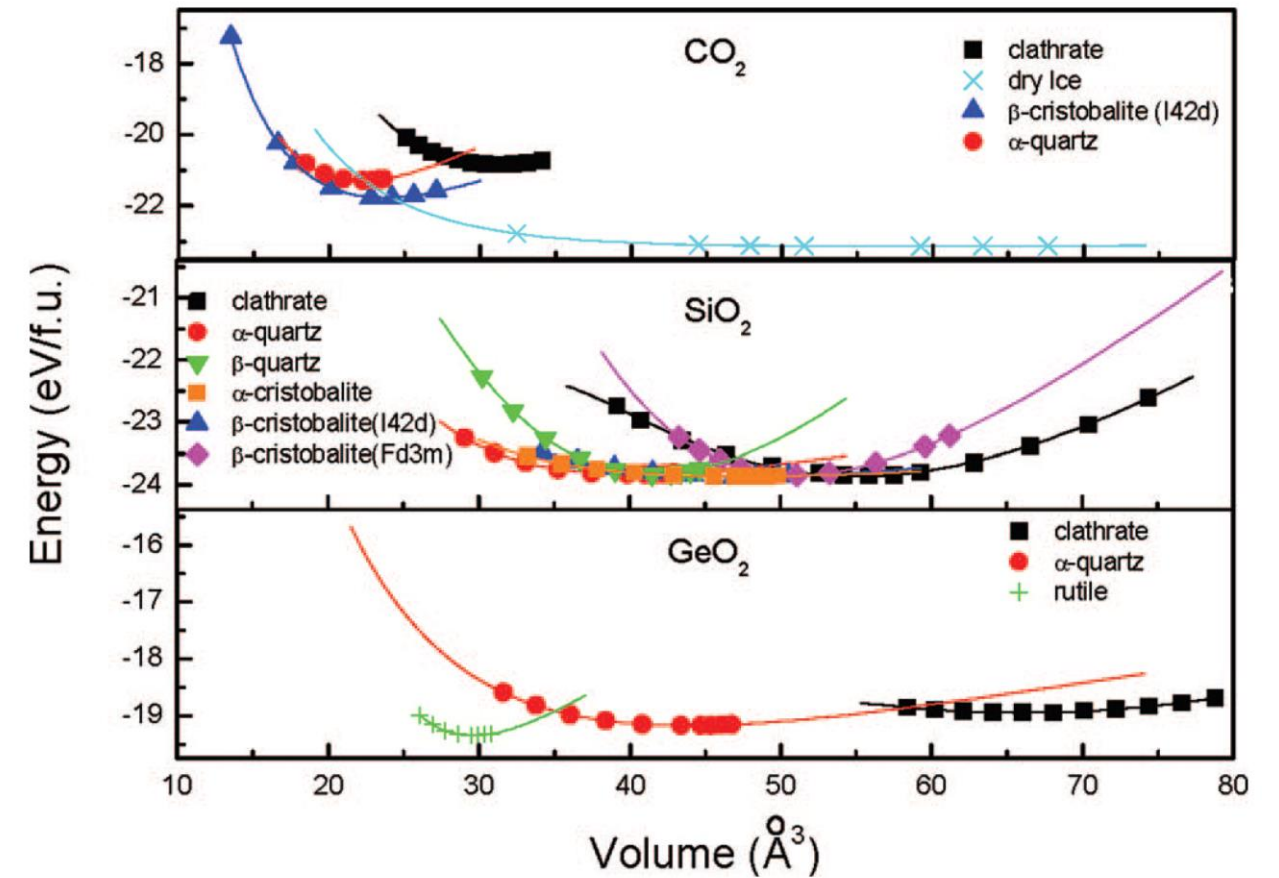


FIG. 2. The energy as function of CO<sub>2</sub>, SiO<sub>2</sub> and GeO<sub>2</sub> volume. The “f.u.” in the y-axis stands for formula unit. I42d stands for  $I\bar{4}2d$ . Fd3m stands for  $Fd\bar{3}m$ .



# Prática 0

---

Primeiro passo: entre no diretório Lab6/Metanol/molecula\_isolada e abra com o seu editor de preferência o *input espresso.in*;

- Utilize o software XCRYSDEN para visualizar a estrutura:
  - digite no terminal xcrysdn;
  - Abra o menu File > Open PWscf > Open PWscf input file
  - selecione seu arquivo de input.
  - observe a estrutura, as posições atômicas da molécula. Gire a estrutura, explore o menu do software