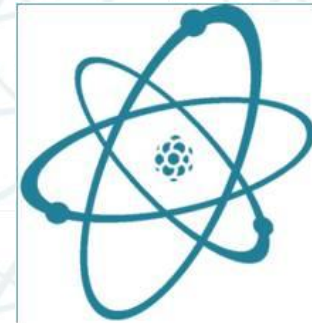


19th Spring Physics Conference, IPM
May 16-17, 2012 (27-28 Ordibehesht 1391)



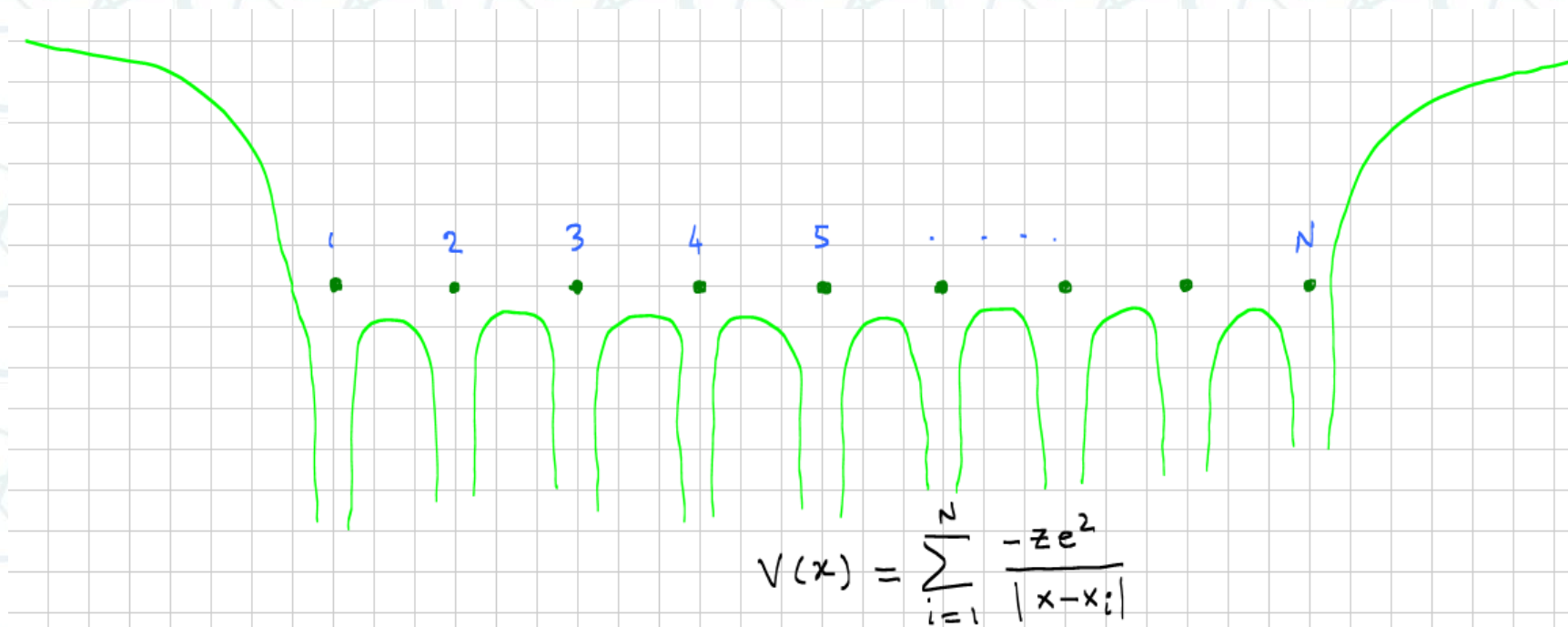
The Jellium Model and its Variants in Electronic Structure Calculations of Materials

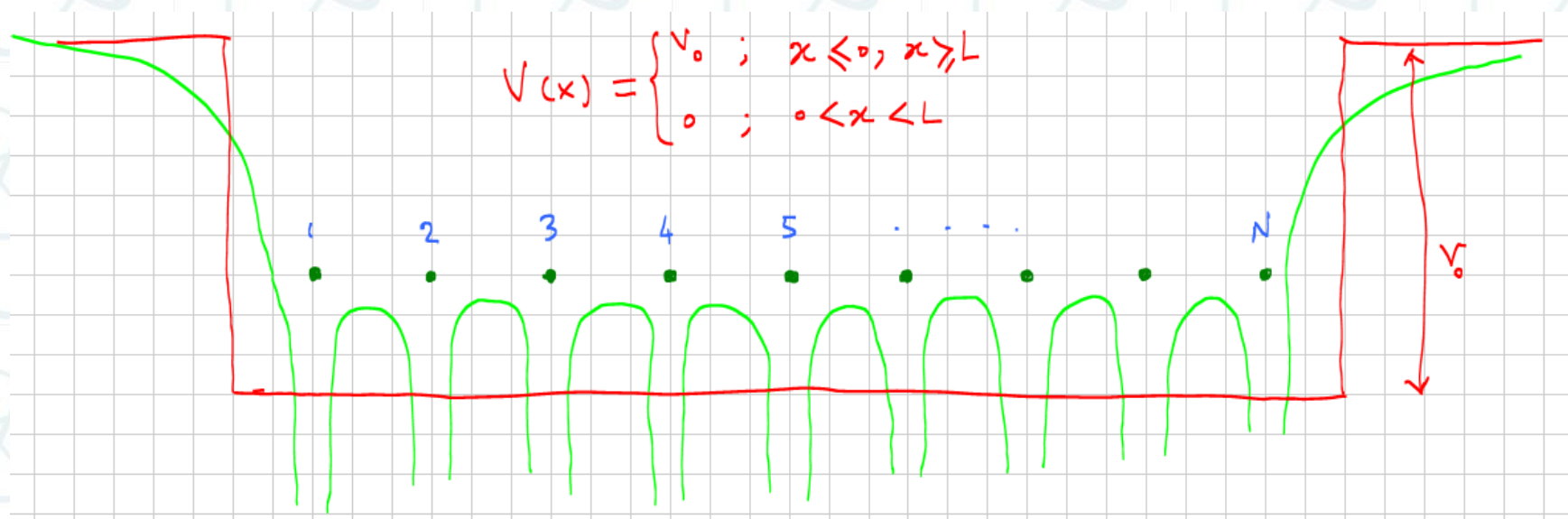
M. Payami

Physics Group, AEOI, Tehran, Iran

[mpayami @ aeoi.org.ir](mailto:mpayami@aeoi.org.ir)

- Calculations based on **simplified models**
- Calculations based on **first-principles methods**



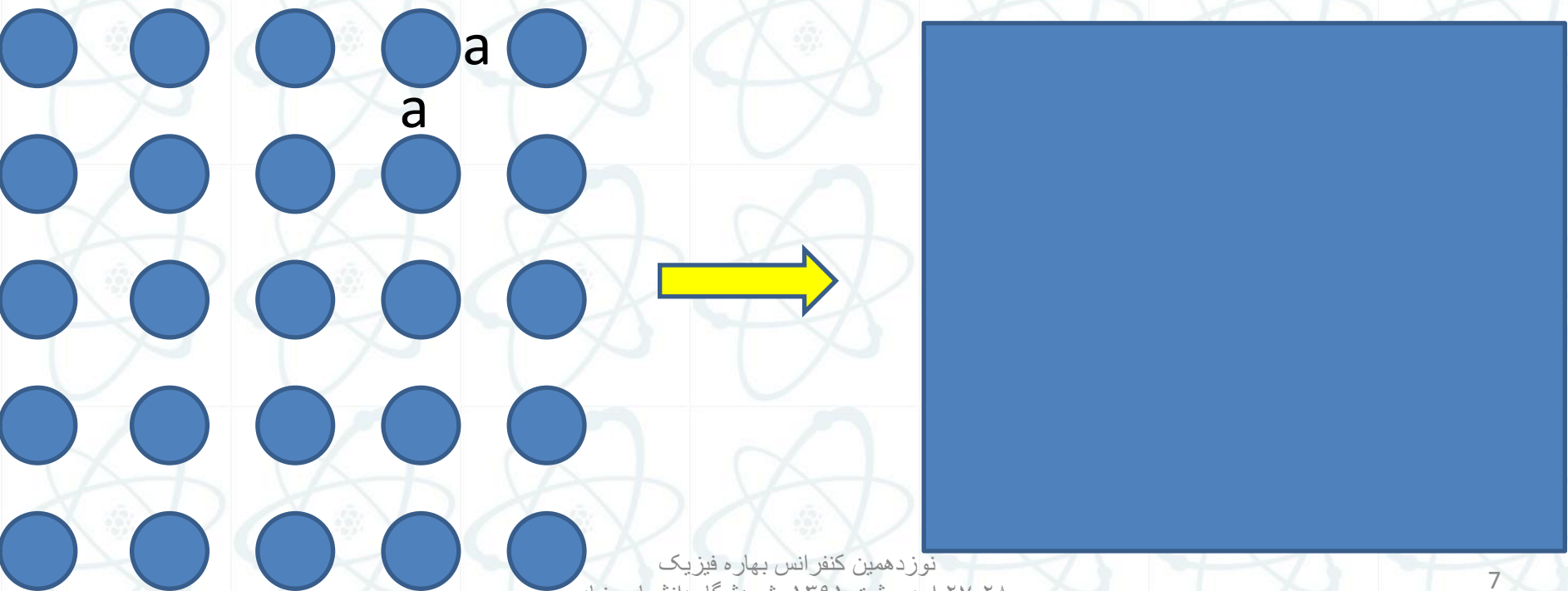


سؤال: این ساده سازی چه مواقعی امکان پذیر است؟

جواب : موافقی که بر هکشن الکترون‌ها و الکترون‌ها با یون‌ها ضعیف باشد
و همچنین خواص الکترونی سیستم به مکان دقیق یون‌ها حس نباشد.

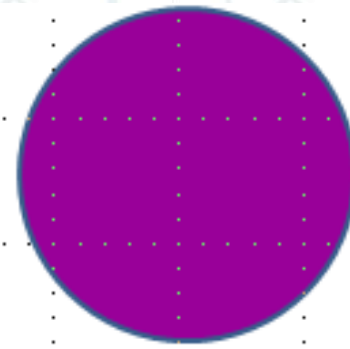
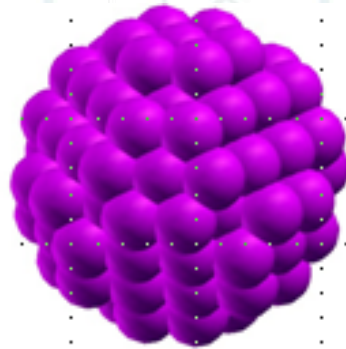
What is Jellium Model (JM)?

- In the simple **JM**, the discrete ions are replaced with a **homogeneous positive background** of density $\bar{n}$



What is Jellium Model (JM)?

- In the simple **JM**, the discrete ions are replaced with a **homogeneous positive background** of density $\bar{n}$



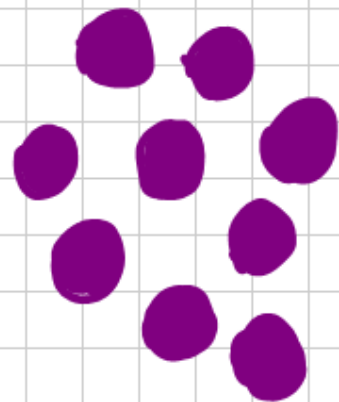
$$n_+(\vec{r}) = \sum_{\vec{R}} \delta(\vec{r} - \vec{R})$$

$$n_+(\vec{r}) = \bar{n} \theta(r_0 - |\vec{r}|)$$
$$\bar{n} = 3 / 4\pi r_s^3$$

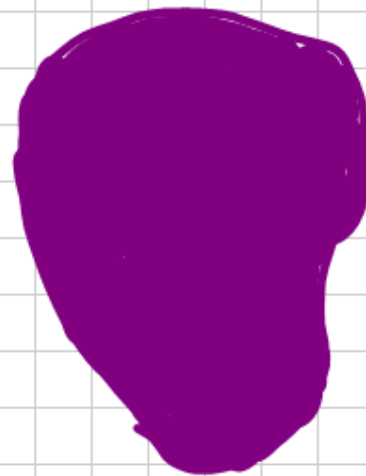
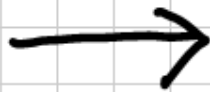
r_s is constant

$$r_0 = z^{1/3} r_s$$
$$r_s = 3.99$$

Jellium Model (JM)



point ions



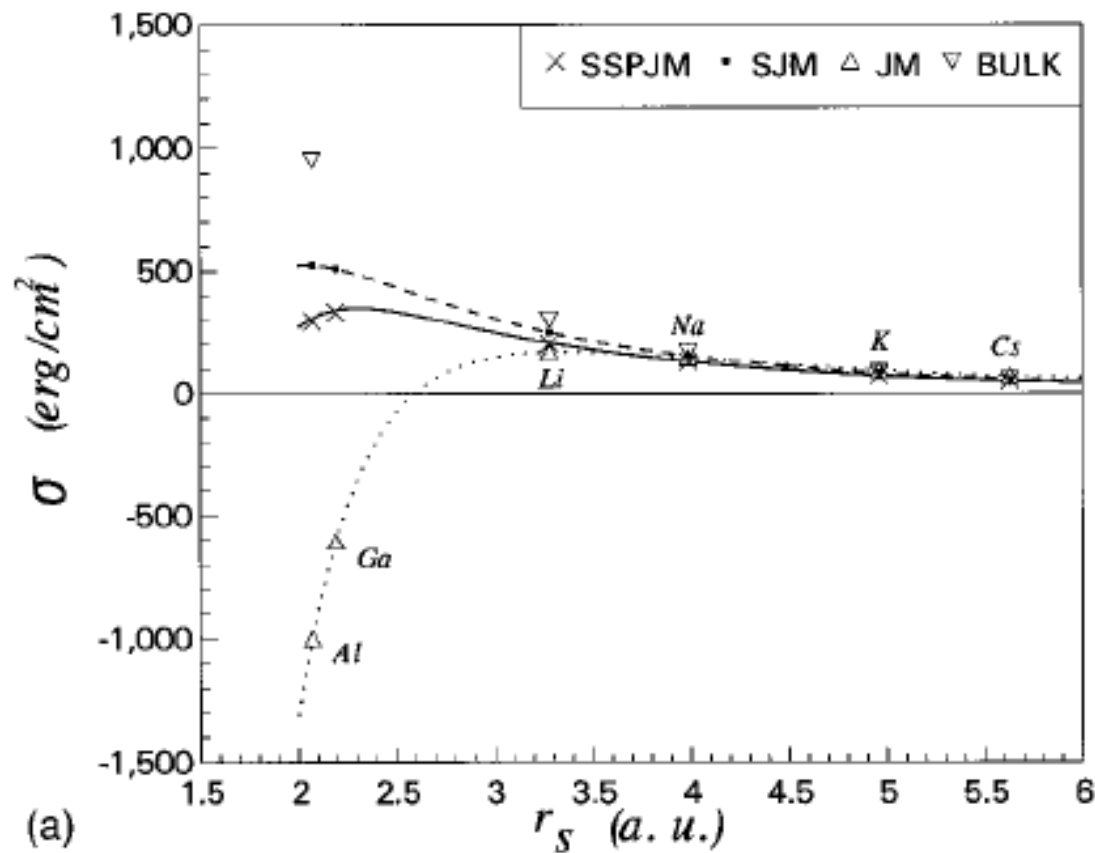
uniform
positive background

Density functional theory

$$E[n, n_+] = T_S[n] + E_{xc}[n] + \\ + \frac{1}{2} \int d\underline{r} \phi([n, n_+]; \underline{r}) [n(\underline{r}) - n_+(\underline{r})]$$

$$\phi(\underline{r}) \equiv \int d\underline{r}' \frac{[n(\underline{r}') - n_+(\underline{r}')] }{|\underline{r} - \underline{r}'|}$$

Application of JM to metal surfaces

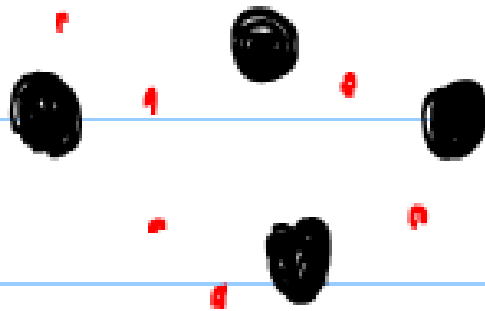


M. Payami and N. Nafari, *J. Chem. Phys.* **109**, 5730-40 (1998)

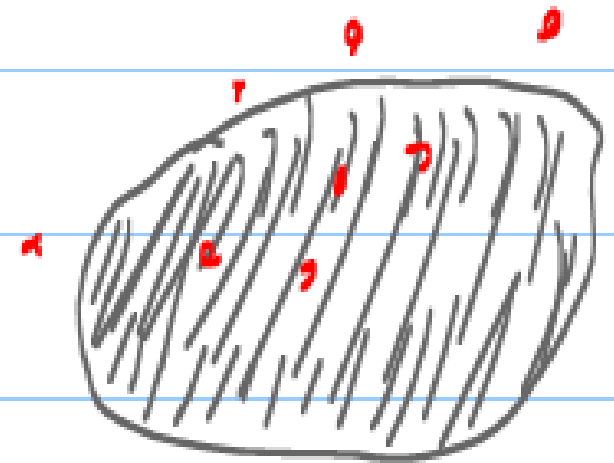
با استفاده از **الگوی شرله ای** برخی از خواص سیستم به خوبی قابل مقایسه
 با نتایج تجربی به دست می آید ولی در برخی موارد ($r_s \leq 2$)
 علامت انرژی سطحی را نادریست می دهند و به ایای $r_s \geq 5$
 مدول حجمی را منفی می دهند .

سؤال: چگونه الگوریتم‌های را اصلاح کنیم تا این مشکلات
نسبتاً برطرف شود؟

واقعی



ساده



Corrections to JM

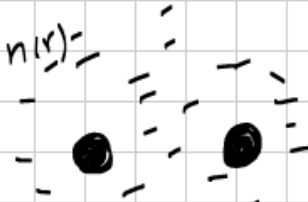
$$E_{\text{pseudo}}[n, \{l\}] = E_{\text{JM}}[n, n_+]$$

$$+ \delta v$$

$$- \text{self-energy of jellium}$$

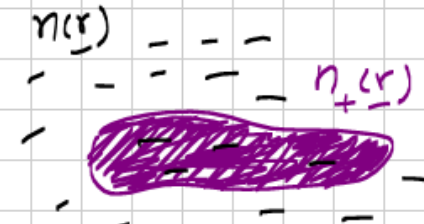
$$E_{\text{pseudo}}[n, \{\underline{\ell}\}] = E_{JM}[n, n_+]$$

$$+ \left(\int d\underline{r} \sum_e W(|\underline{r} - \underline{\ell}|) n(\underline{r}) - \frac{1}{2} \int d\underline{r} d\underline{r}' \frac{n_+(\underline{r}) n(\underline{r}')}{|\underline{r} - \underline{r}'|} \right) \\ - \left(\frac{1}{2} \int \frac{n_+(\underline{r}) n_+(\underline{r}')}{|\underline{r} - \underline{r}'|} d\underline{r} d\underline{r}' - \frac{1}{2} \sum_{\underline{\ell}, \underline{\ell}'} \frac{z^2}{|\underline{\ell} - \underline{\ell}'|} \right)$$



A diagram showing two black dots representing point charges. Dashed lines radiate from each dot, representing electric field lines. The label $n(\underline{r})$ is written above the left dot.

$$E_{e-i} = \int n(\underline{r}) \left[\sum_{\underline{l}} \frac{-ze^2}{|\underline{r} - \underline{l}|} \right] d\underline{r}$$



A diagram showing a purple shaded, elongated region representing a charge distribution. Dashed lines radiate from the region. The label $n(\underline{r})$ is written above the left side, and $n_+(\underline{r})$ is written above the right side.

$$E_{e-b} = -e^2 \int \frac{n(\underline{r}) n_+(\underline{r}')}{|\underline{r} - \underline{r}'|} d\underline{r} d\underline{r}'$$



$$E_{i-i} = \frac{1}{2} \sum_{\substack{\underline{l} \neq \underline{l}' \\ \sim \sim}} \frac{(Ze)^2}{|\underline{l} - \underline{l}'|}$$

JM



$$E_{b-b} = \frac{e^2}{2} \int \frac{n_+(\underline{r}) n_+(\underline{r}')}{|\underline{r} - \underline{r}'|}$$

$$W(r) = -\frac{Z}{r} + W_R(r)$$

$$W_R(r) = +\frac{Z}{r} \Theta(r_c - r)$$

core radius

Ashcroft
empty-core
pseudo-pot.

Stabilized jellium model **SJM**

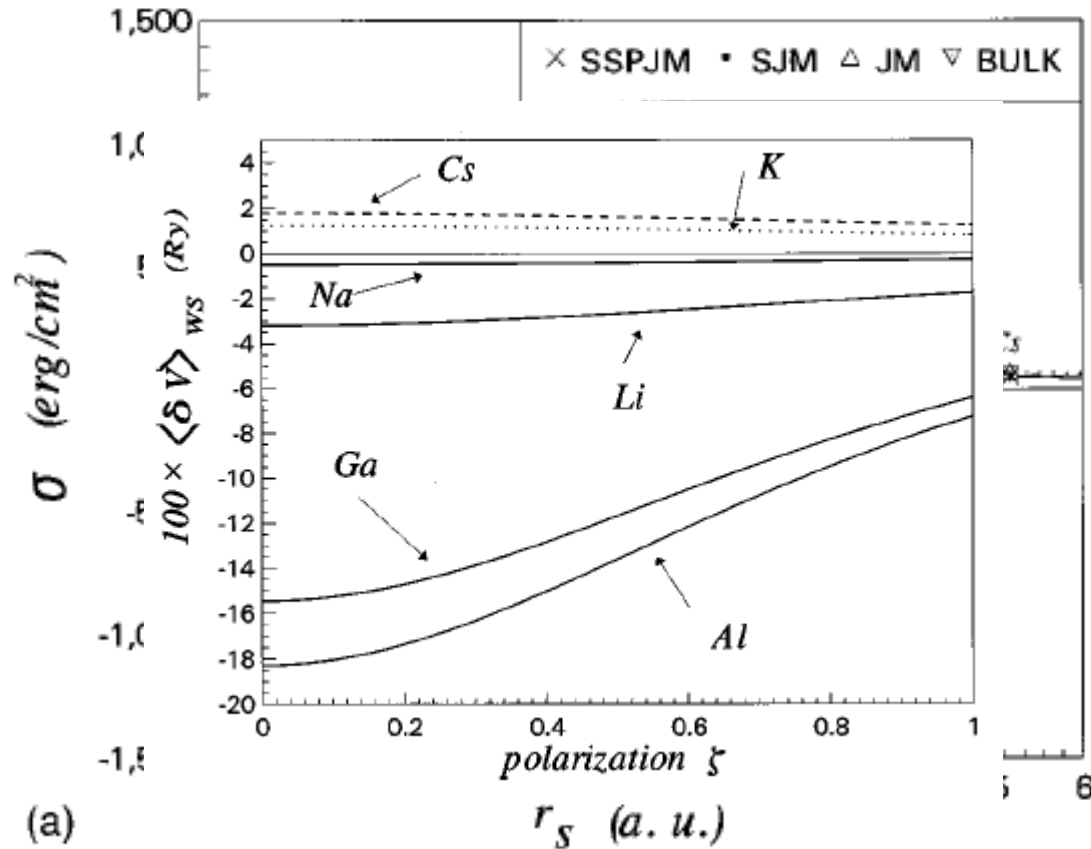
$$\text{SJM:} \left\{ \begin{array}{l} \delta v \approx \langle \delta v \rangle_{ws} \oplus (r) \\ \text{self-energy} \approx N \tilde{\epsilon} \quad ; \quad \tilde{\epsilon} = \frac{3Z}{5r_0} \end{array} \right.$$

SJM energy functional

$$\begin{aligned} E_{\text{SJM}}[n, n_+] &= E_{\text{JM}}[n, n_+] \\ &+ \langle \delta v \rangle_{\text{WS}} \int [n(\underline{r}) - n_+(\underline{r})] d\underline{r} \\ &+ (\bar{W}_R(\bar{n}) + \varepsilon_M(\bar{n})) \int d\underline{r} n_+(\underline{r}) \end{aligned}$$

J. P. Perdew, H. Q. Tran, E. D. Smith, *Phys. Rev. B* **42**, 11627 (1990)

Application of **SJM** to metal surfaces



M. Payami and N. Nafari, *J. Chem. Phys.* **109**, 5730-40 (1998)

Spin-polarized EG

$$\varepsilon(r_s, \zeta) = t_s(r_s, \zeta) + \varepsilon_x(r_s, \zeta) + \varepsilon_c(r_s, \zeta)$$

به ازای قطبش مشخص، چه
موقع سیستم متعادل است؟

Equilibrium condition for EG

$$0 = P(\bar{n}, \zeta) = - \left(\frac{\partial E}{\partial V} \right)_{N, \zeta} = \bar{n}^2 \left(\frac{\partial}{\partial n} \right)_{\zeta} \varepsilon(\bar{n}, \zeta)$$

$$= - \frac{1}{4 \pi \bar{r}_s^2} \left(\frac{\partial}{\partial r_s} \right)_{\zeta} \varepsilon(\bar{r}_s, \zeta).$$

$$0 = \frac{1}{4 \pi r_s^2} \left\{ \frac{2}{r_s} t_s(r_s, \zeta) + \frac{1}{r_s} \varepsilon_x(r_s, \zeta) - \left(\frac{\partial}{\partial r_s} \right)_{\zeta} \varepsilon_c(r_s, \zeta) \right\}$$

$$\bar{r}_s^{\text{EG}}(\zeta) = 4.18 + \Delta r_s^{\text{EG}}$$

Generalization to any metal

$$\overline{r}_s^X(\zeta) = \overline{r}_s^X(0) + \Delta \overline{r}_s^{\text{EG}}$$

X= Ga, Al, Li, Na, K, Cs

Stabilized spin-polarized JM

$$n_{\uparrow} = \frac{1}{2}(1 + \zeta)n, \quad n_{\downarrow} = \frac{1}{2}(1 - \zeta)n$$

$$\varepsilon(n, \zeta) = t_s(n, \zeta) + \varepsilon_{xc}(n, \zeta) + \overline{w}_R(n, r_c) + \varepsilon_M(n) + \varepsilon_{bs},$$

where

$$t_s(n, \zeta) = \frac{1}{2} c_k [(1 + \zeta)^{5/3} + (1 - \zeta)^{5/3}] n^{2/3},$$

$$\varepsilon_{xc}(n, \zeta) = \frac{1}{2} c_x [(1 + \zeta)^{4/3} + (1 - \zeta)^{4/3}] n^{1/3} + \varepsilon_c(n, \zeta),$$

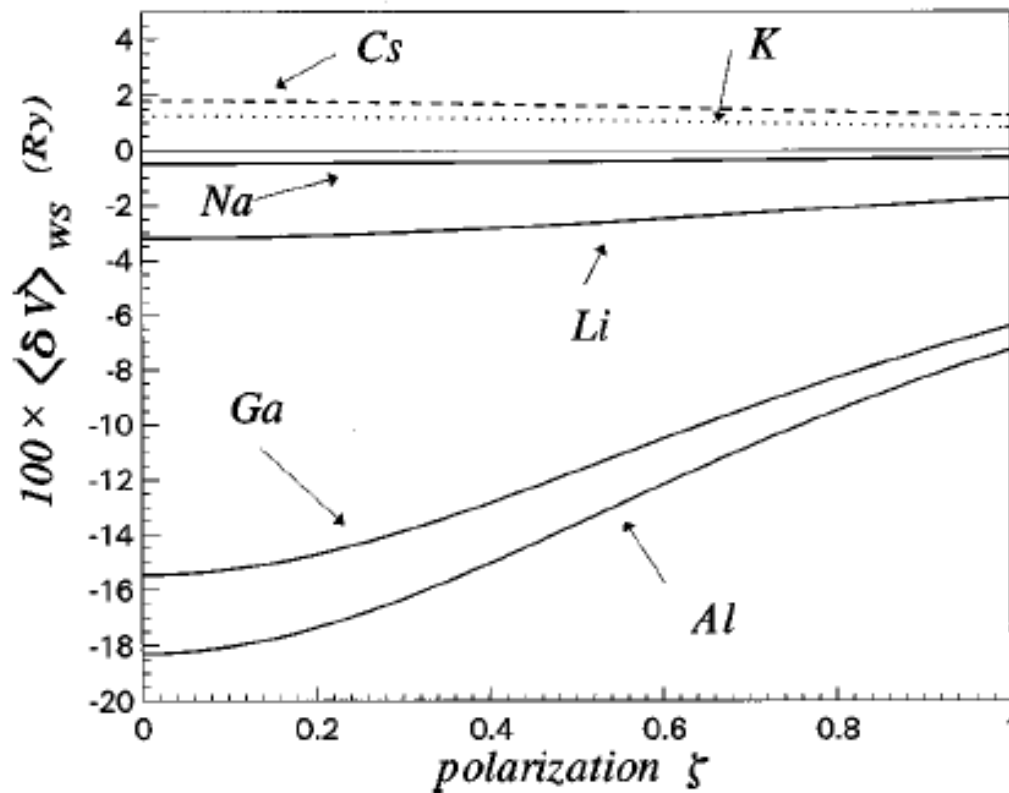
$$c_k = \frac{3}{5} (3 \pi^2)^{2/3}; \quad c_x = \frac{3}{2} \left(\frac{3}{\pi} \right)^{1/3}.$$

Equilibrium condition for SSPJM

$$2t_s(\bar{r}_s, \xi) + \varepsilon_x(\bar{r}_s, \xi) - \bar{r}_s \left(\frac{\partial}{\partial r_s} \right)_{\xi} \varepsilon_c(\bar{r}_s, \xi) + \frac{9}{r_s^3} r_c^2 + \varepsilon_M(\bar{r}_s) = 0.$$

r_c as a function of r_s and zeta

Polarization dependence of $\langle \delta v \rangle$

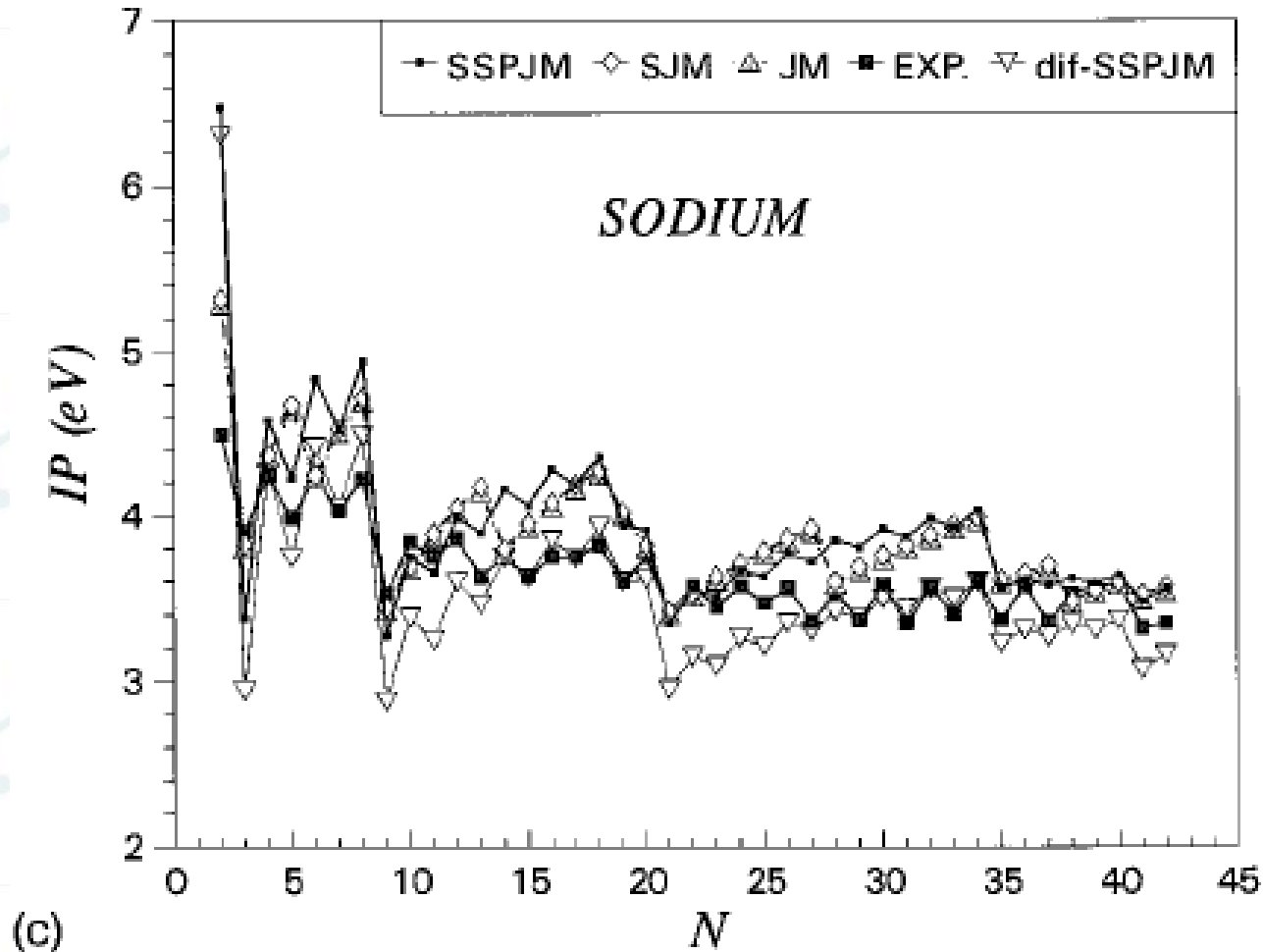


M. Payami and N. Nafari, *J. Chem. Phys.* **109**, 5730-40 (1998)

Energy functional in SSPJM

$$\begin{aligned} E_{\text{SSPJM}}[n_{\uparrow}, n_{\downarrow}, n_{+}] \\ = E_{\text{JM}}[n_{\uparrow}, n_{\downarrow}, n_{+}] + (\varepsilon_M(\bar{n}) + \bar{w}_R(\bar{n}, \xi)) \int d\mathbf{r} n_{+}(\mathbf{r}) \\ + \langle \delta v \rangle_{\text{WS}}(\bar{n}, \xi) \int d\mathbf{r} \Theta(\mathbf{r}) [n(\mathbf{r}) - n_{+}(\mathbf{r})], \end{aligned}$$

Application of SSPJM to metal clusters



(c)

SSPJM

- **Stabilized Spin-Polarized Jellium Model and Odd-Even Alternations in Jellium Metal Clusters**, M. Payami and N. Nafari, J. Chem Phys. 109, 5730 (1998)
- **Finite-size effects and the stabilized spin-polarized jellium model for metal clusters**, M. Payami, J. Chem. Phys. 111, 8344 (1999)
- **Volume change of bulk metals and metal clusters due to spin-polarization**, M. Payami, J. Phys.: Condens. Matter 13, 4129 (2001)
- **Equilibrium sizes of jellium metal clusters in the stabilized spin-polarized jellium model**, M. Payami, Phys. Stat. Sol. (b) 225, 77 (2001)

Self-compressed SJM

- Finite systems are not stable in SJM

J. P. Perdew, M. Brajczewska, and C. Fiolhais, Solid State Commun. 88, 795 (1993)

SC-SJM Energy functional

$$\begin{aligned} E_{\text{SC-SJM}}[n, \bar{n}] &= E_{\text{JM}}[n, \bar{n}] \\ &+ \langle \delta v \rangle_{\text{WS}} \int [n_-(\underline{r}) - n_+(\underline{r})] d\underline{r} \\ &+ (\bar{W}_R(\bar{n}) + \epsilon_M(\bar{n})) \int d\underline{r} n_+(\underline{r}) \end{aligned}$$

Let $\bar{n}$ change until the energy minimize

SC-SJM

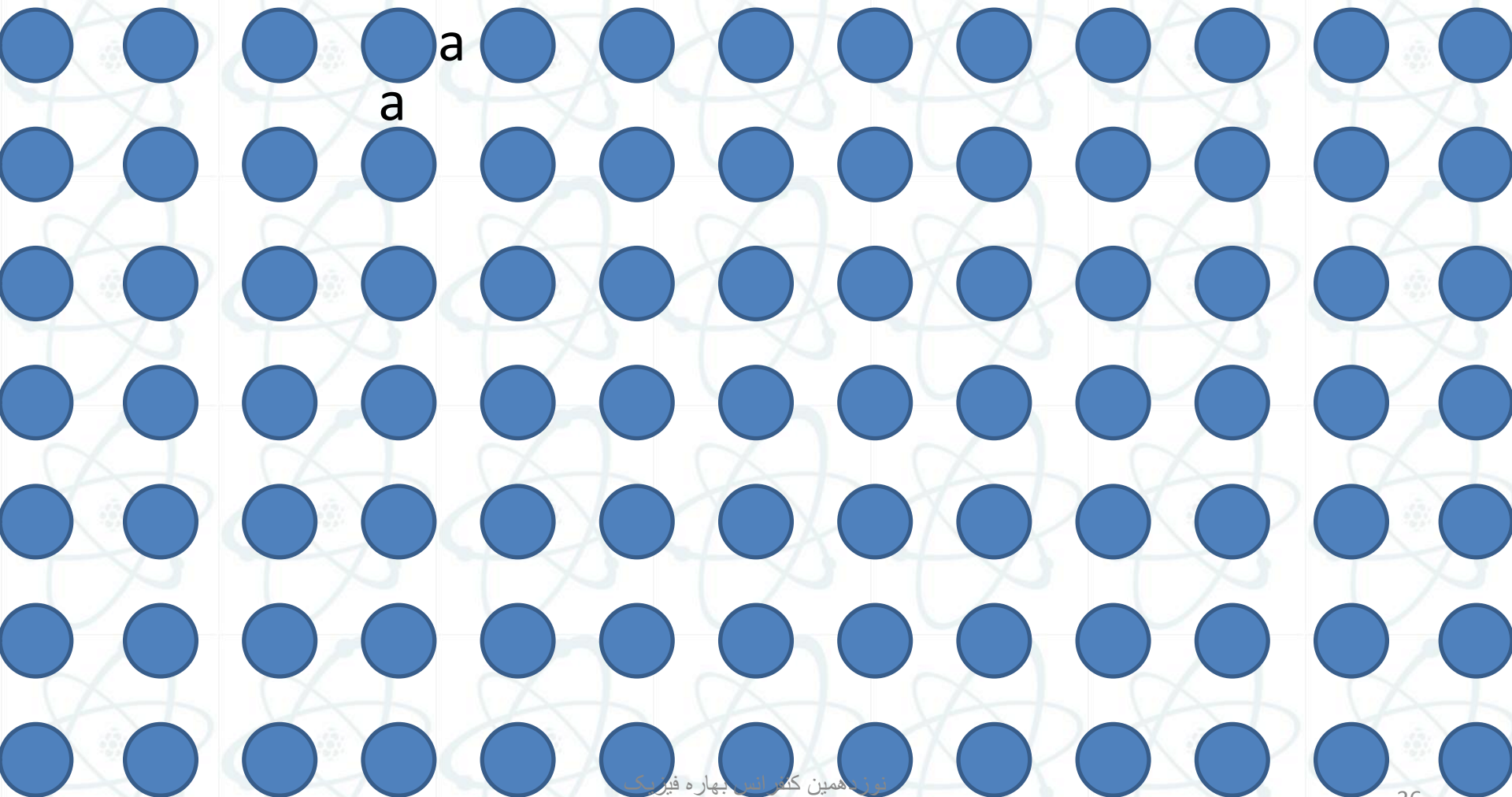
$$E_{SC-SJM} = E_{SJ M}[n, \bar{n}^{\dagger}]$$

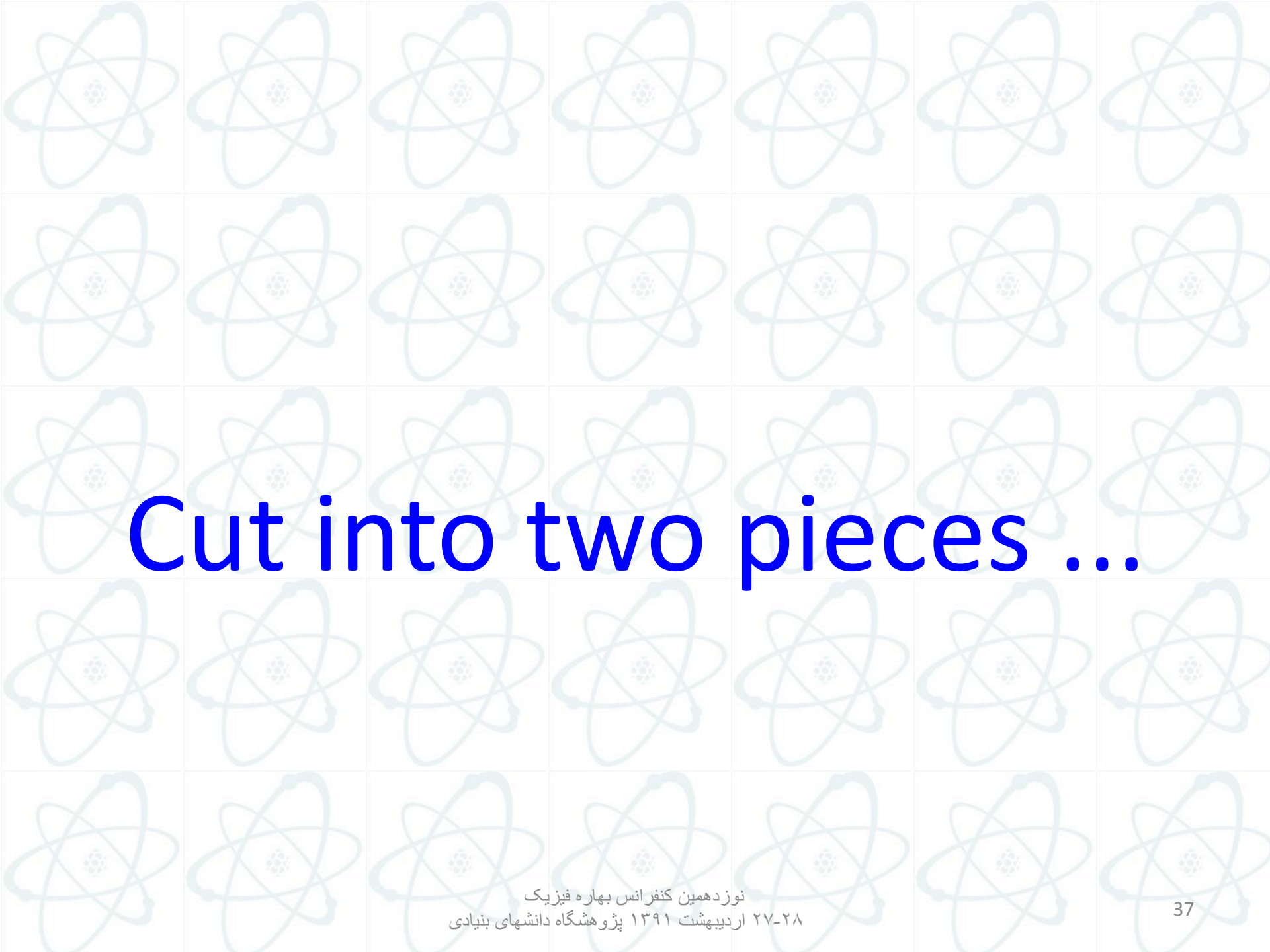
$$\frac{\partial E[n, \bar{n}]}{\partial \bar{n}} \bigg|_{\bar{n}^{\dagger}} = 0$$

SC-SJM

- **Fragmentation of positively charged metal clusters in stabilized jellium model with self-compression**, M. Payami, arXiv:physics/0112022
- **Study of interaction of high-power Ar^{+} laser beam with Ag^{+} -doped glass**, A. Nahal, H. R. M. Kholesifard, M. Payami, arXiv:physics/0302073
- **Stabilized jellium model and structural relaxation effects on the fragmentation energies of ionized silver clusters**, M. Payami, Can. J. Phys. 82, 239 (2004)
- **Fragmentation of multiply charged simple metal clusters in liquid-drop stabilized jellium model**, M. Payami, Phys. Stat. Sol. (b) 241, 1838 (2004)
- **Self-consistent iterative solution of the exchange-only OEP equations for simple metal clusters in jellium model**, M. Payami, T. Mahmoodi, J. Phys.: Condens. Matter Vol 18, 75 (2006)
- **Exact exchange optimized effective potential and self-compression of stabilized jellium clusters**, M. Payami, Phys. Rev. B 73, 113106 (2006)
- **Equilibrium properties of simple metal thin films in the self-compressed stabilized jellium model**, T. Mahmoodi, M. Payami, J. Phys.: Condens. Matter 21, 265002 (2009)

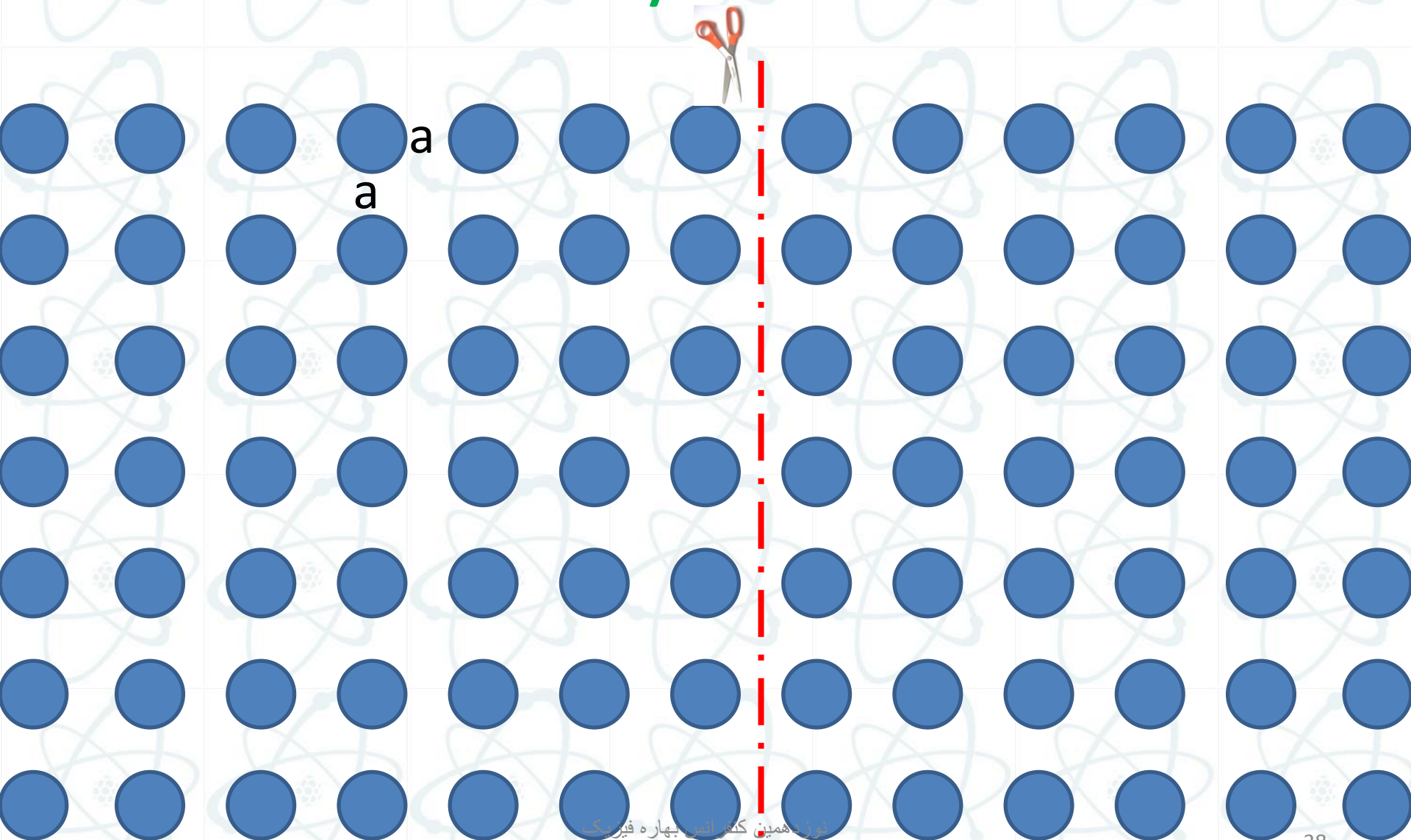
Infinite Crystalline Solid

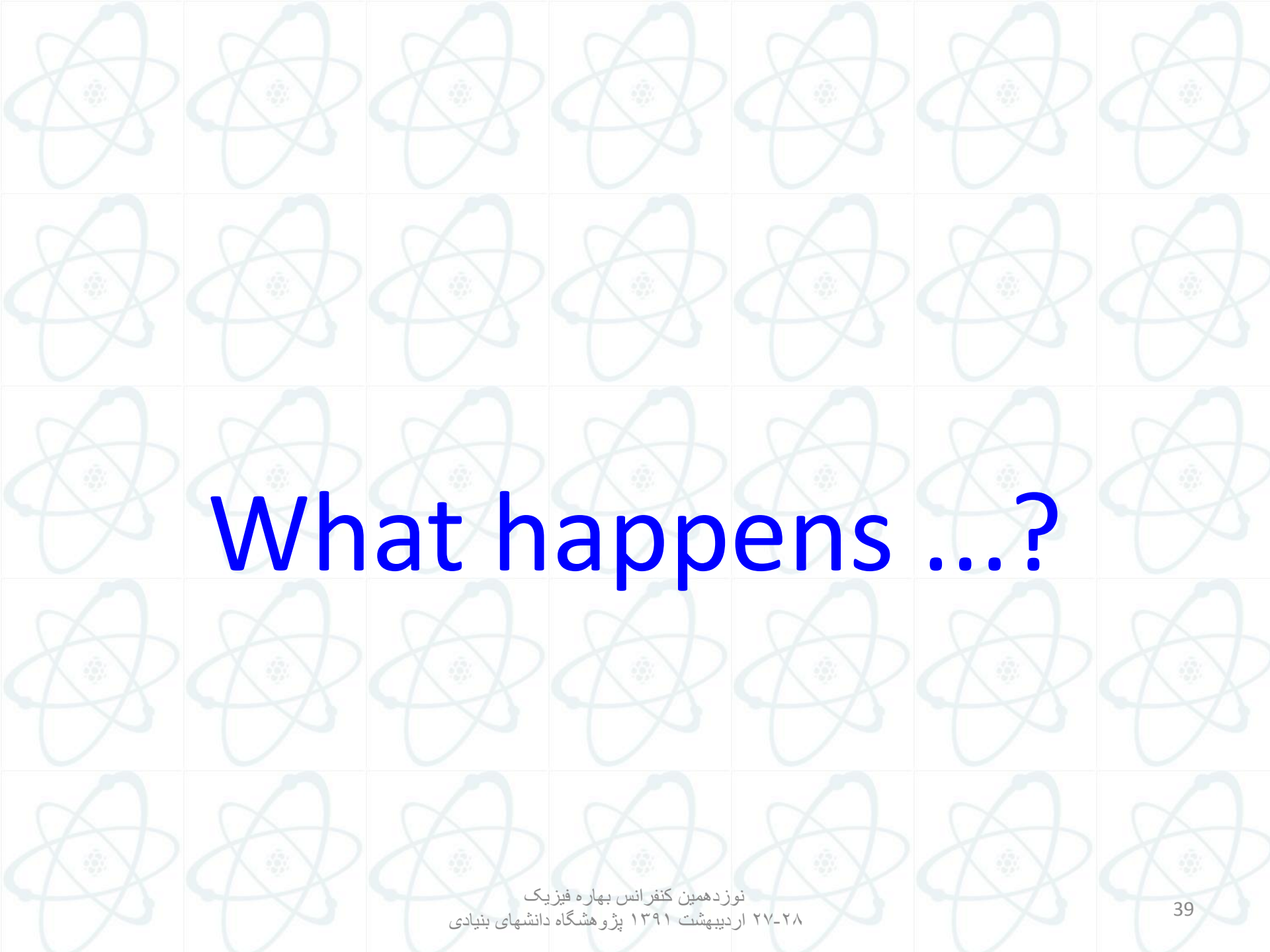




Cut into two pieces ...

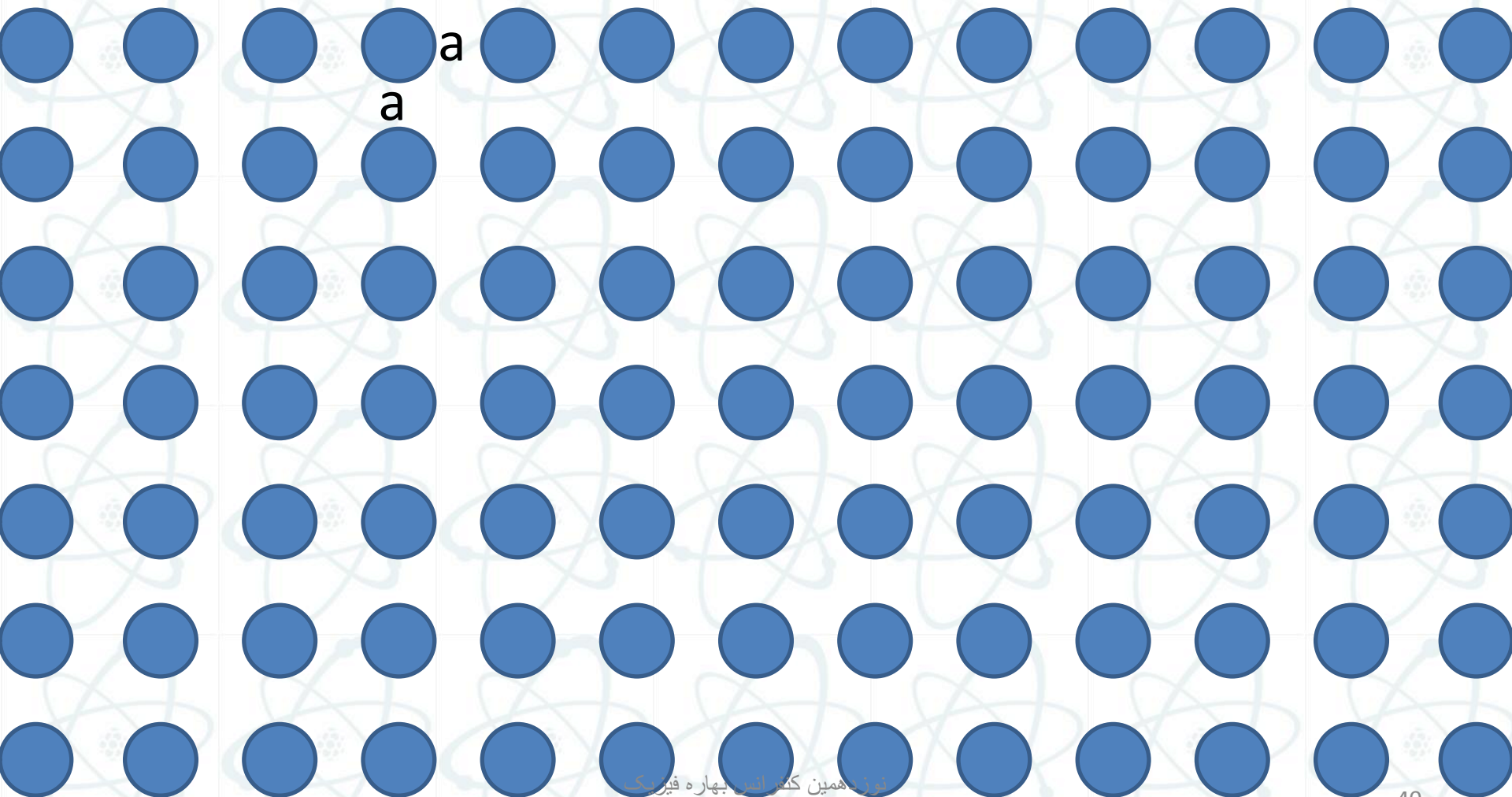
Infinite Crystalline Solid



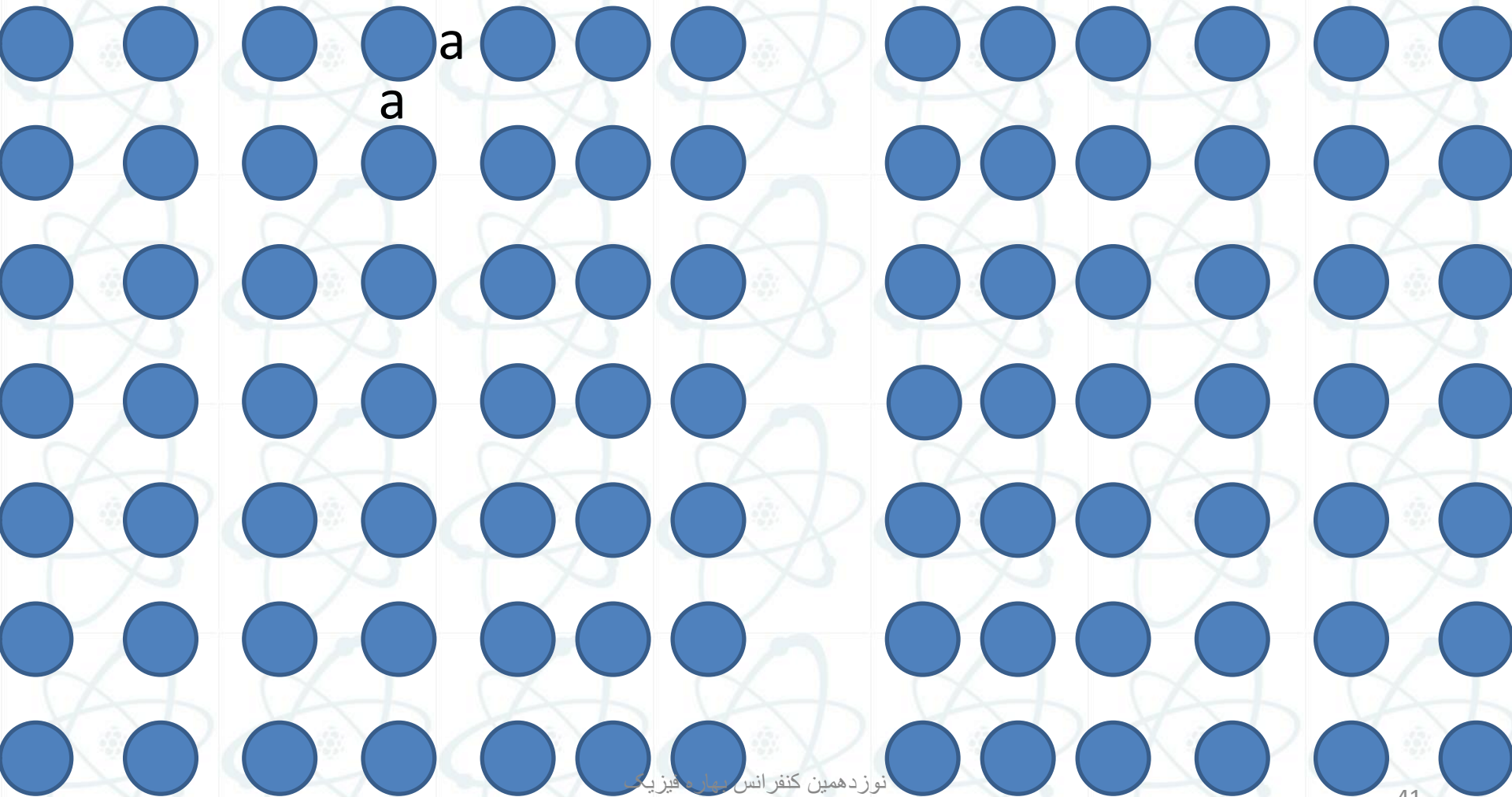


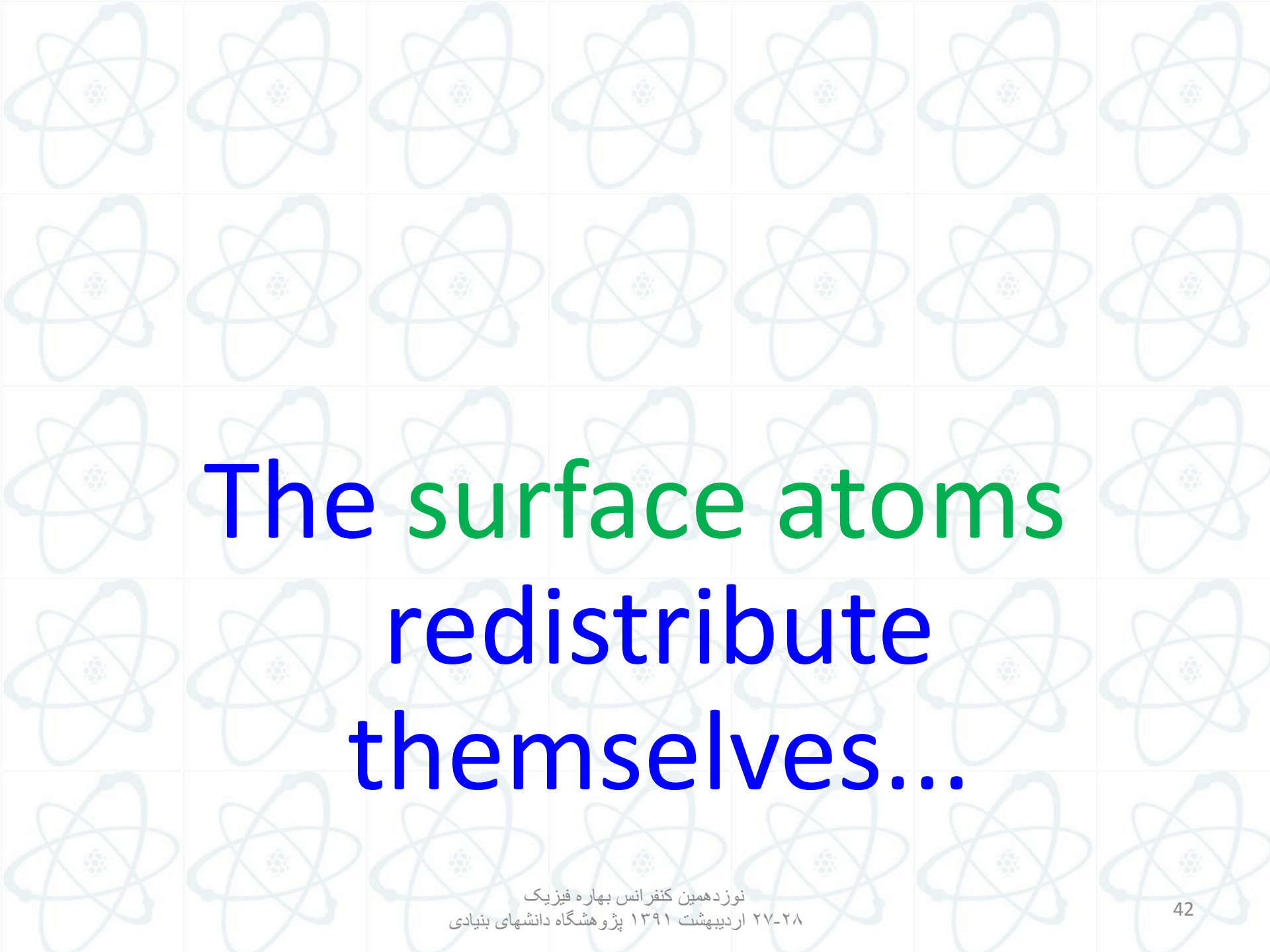
What happens ...?

Infinite Crystalline Solid



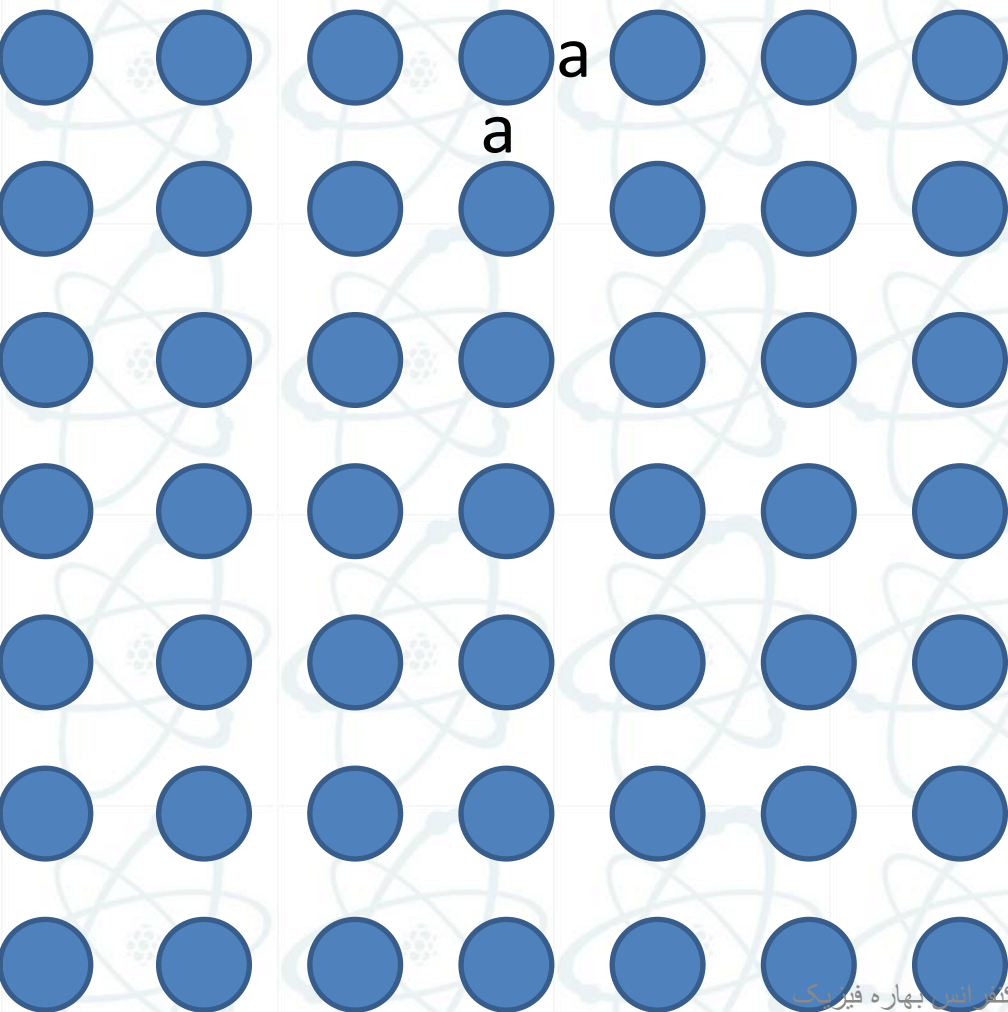
Two Semi-Infinite Crystalline Solid



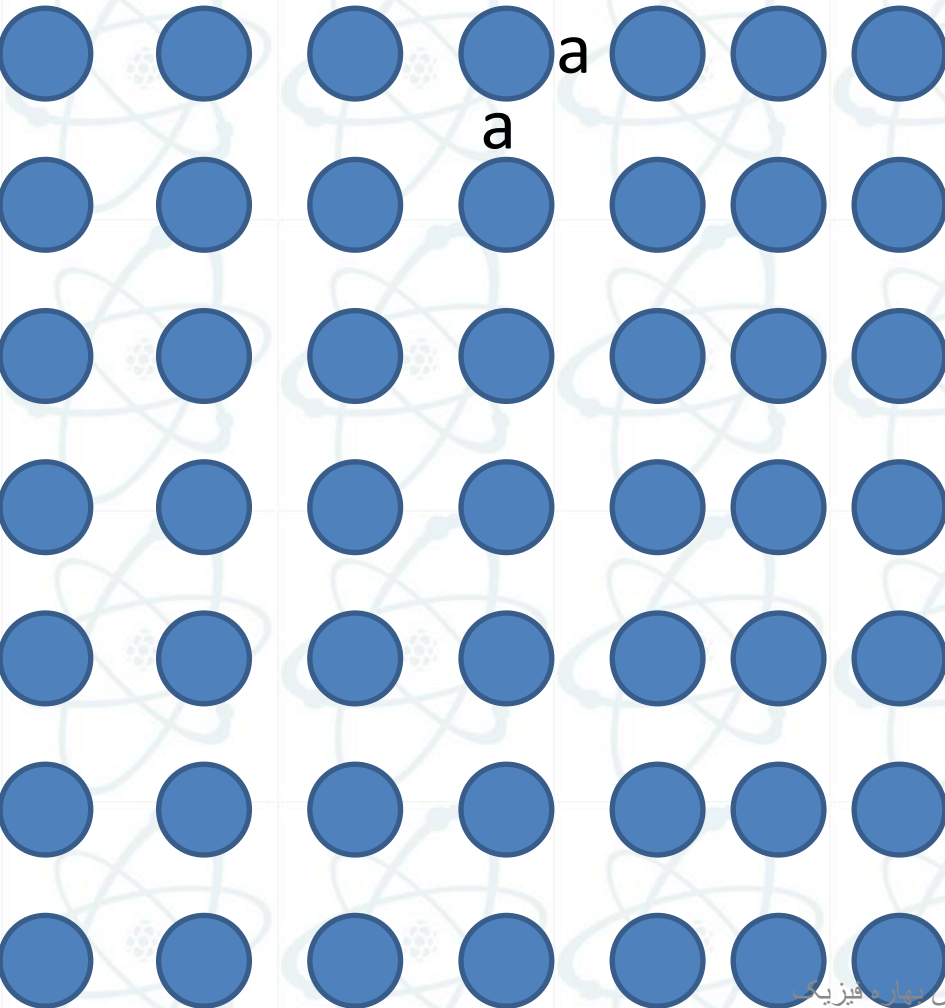
The background of the slide is a repeating pattern of stylized atoms. Each atom consists of a central nucleus, represented by a cluster of small dots, and two elliptical orbits, one horizontal and one vertical, intersecting at the nucleus. The atoms are light blue and are arranged in a grid-like fashion across the entire slide.

The surface atoms redistribute themselves...

Semi-Infinite Crystalline Solid



Semi-Infinite Crystalline Solid

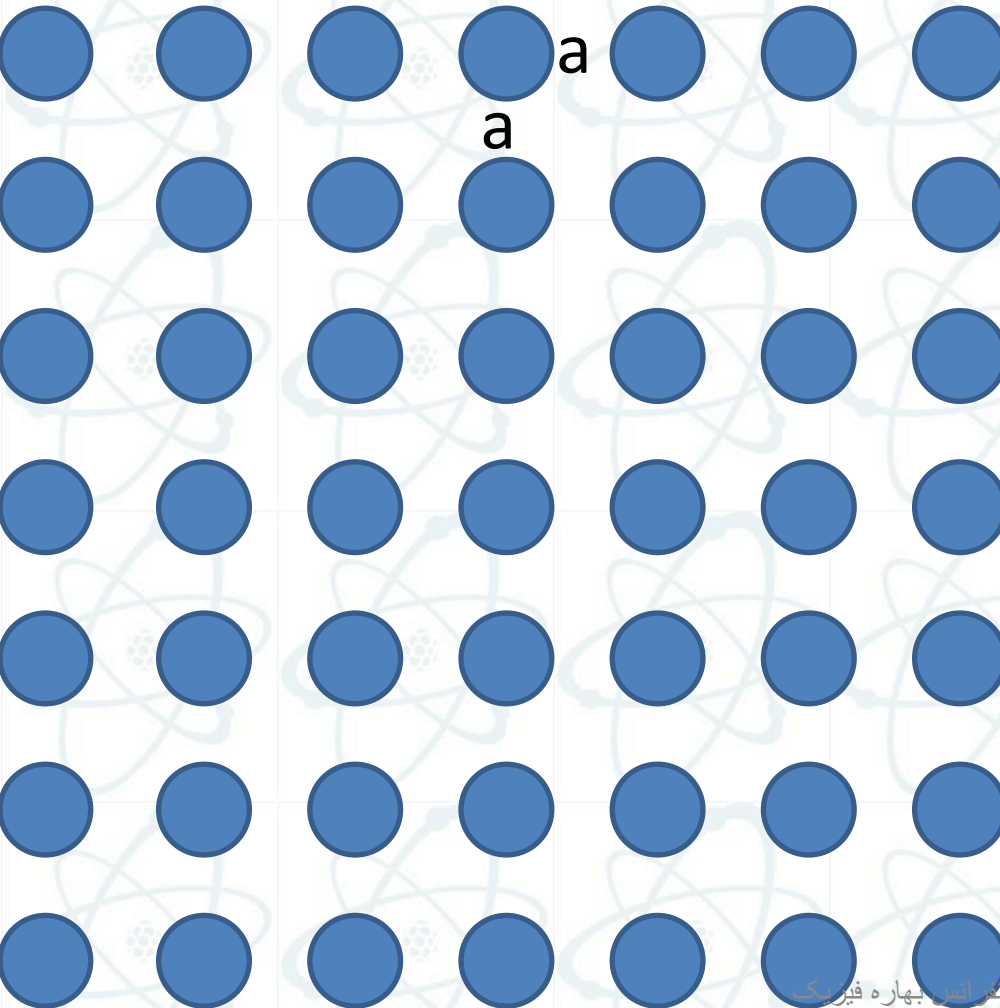


- Near the surface of a semi-infinite crystal, the interatomic distances are different from those in the bulk.
- That is: the ionic density in surface region is different from that in the bulk region.

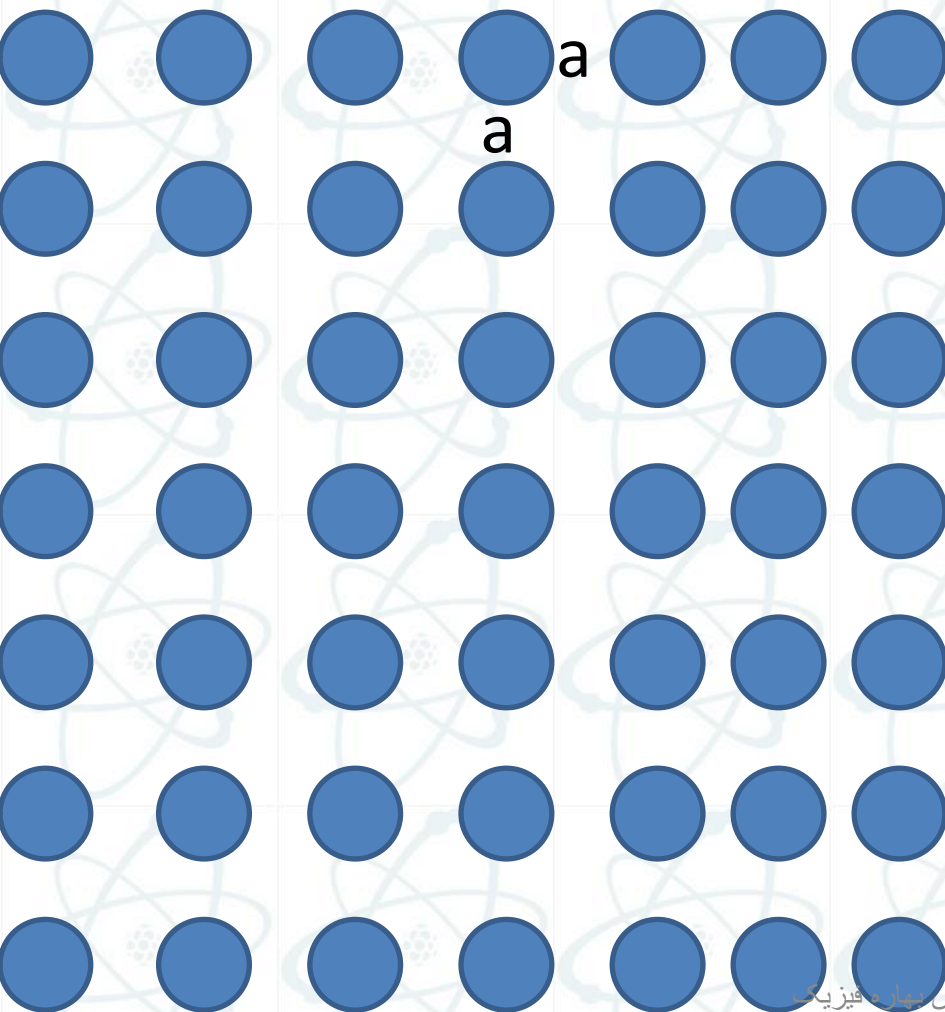




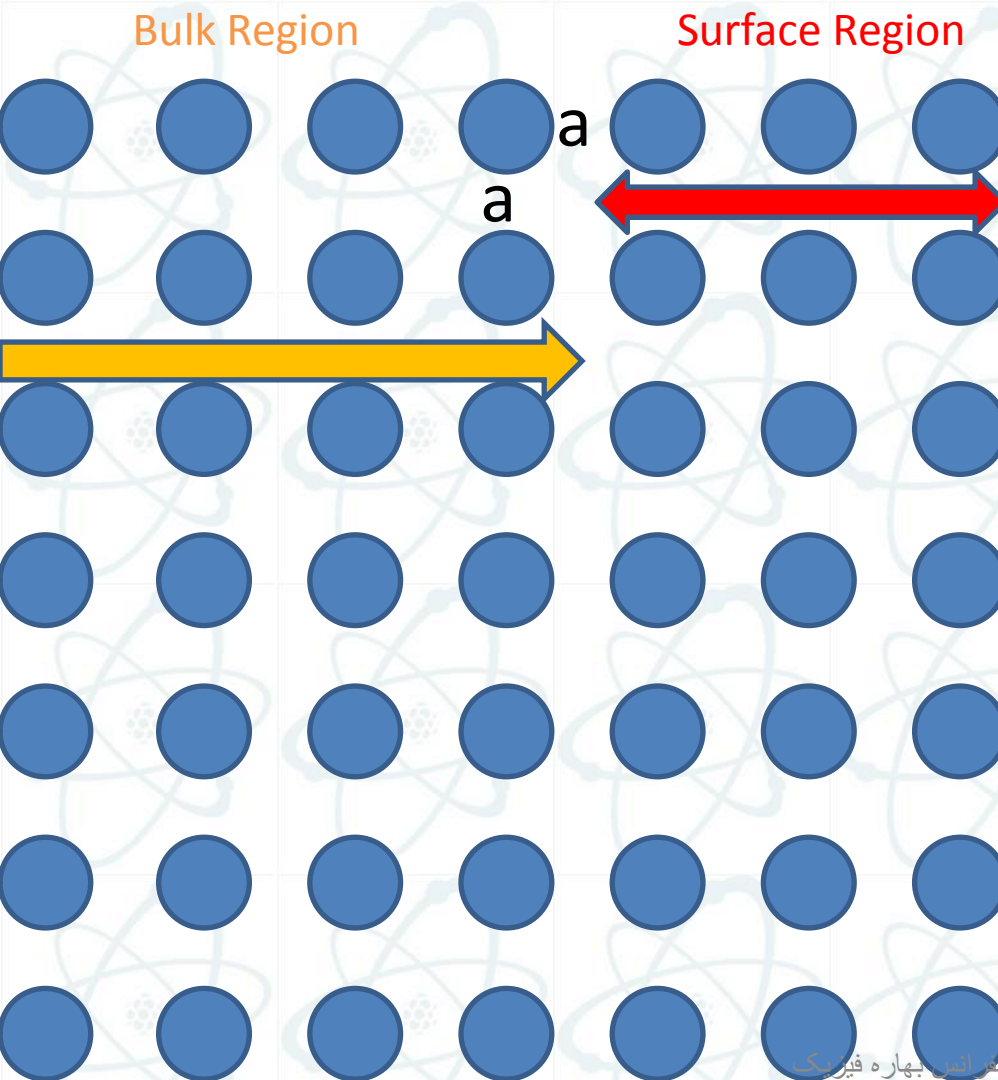
Semi-Infinite Crystalline Solid



Semi-Infinite Crystalline Solid



Semi-Infinite Crystalline Solid



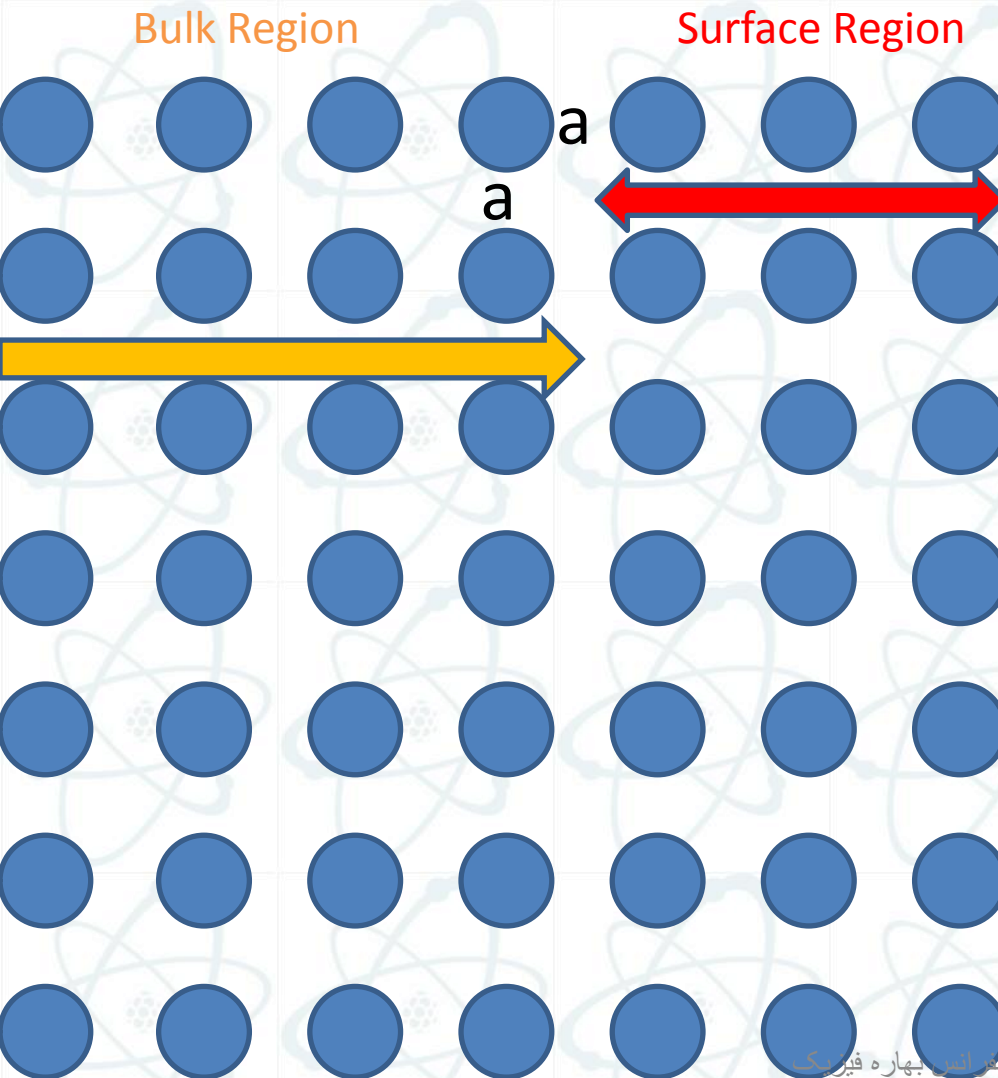
- How many atomic layers in the **surface region**?
- Surface Region: **Expansion** or **Contraction**?

To answer these questions, we
have formulated:

**Self-compressed inhomogeneous
stabilized jellium model (SC-ISJM)**

M. Payami, T. Mahmoodi, *Can. J. Phys.* **89**, 967
(2011).

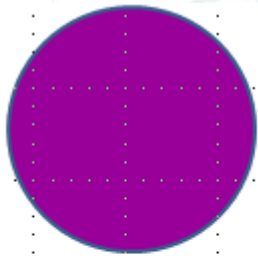
Semi-Infinite Crystalline Solid



- How many atomic layers in the **surface region**?
- Surface Region: **Expansion** or **Contraction**?

SC-SJM

- In Self-Compressed Stabilized Jellium Model (SC-SJM) :



$$n_+(\vec{r}) = \bar{n} \theta(r_0 - |\vec{r}|)$$
$$\bar{n} = 3 / 4 \pi r_s^3$$
$$r_0 = z^{1/3} r_s$$

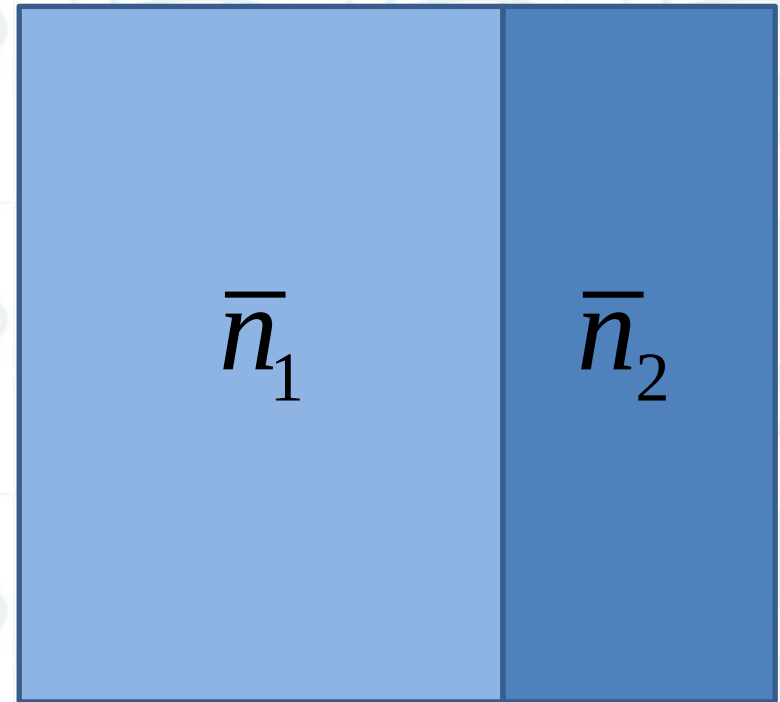
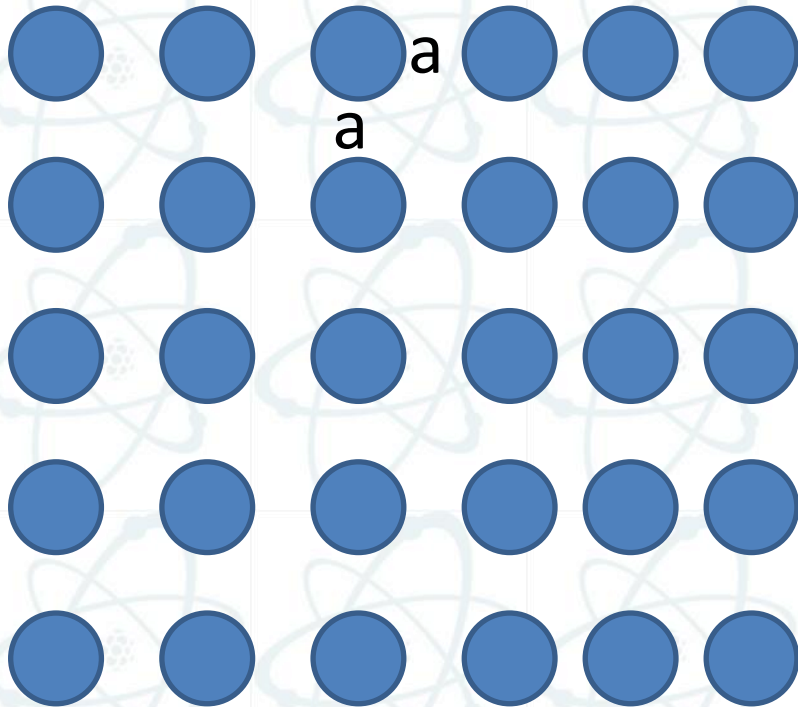
Energy minimization determines r_s :

$$\partial E / \partial r_s \Big|_{r_s^\dagger} = 0$$

$r_s^\dagger$ determines the equilibrium density

r_s is variable

Inhomogeneous Jellium Model



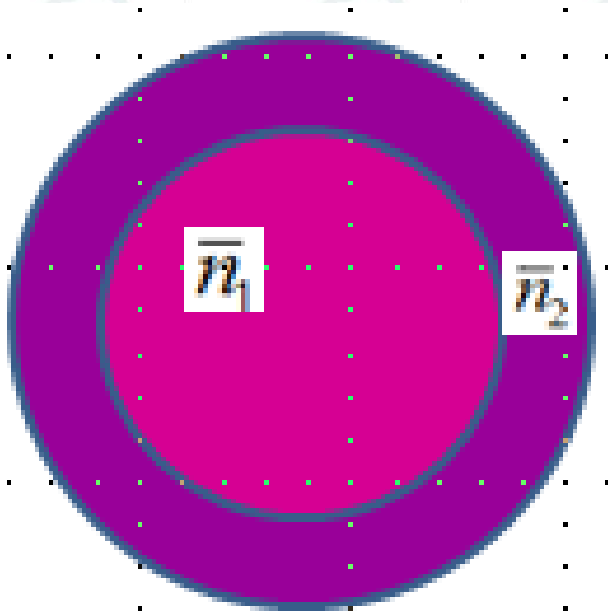
SC-ISJM

- In Self-Compressed Inhomogeneous Stabilized Jellium Model:

$\bar{n}_1$ and $\bar{n}_2$ are variables

$$\partial E / \partial \bar{n}_1 \Big|_{\bar{n}_1 \uparrow} = 0$$

$$\partial E / \partial \bar{n}_2 \Big|_{\bar{n}_2 \uparrow} = 0$$



ISJM

$$E_{ISJM}[n, \{n_+^{(\alpha)}\}] = E_{JM}[n, \{n_+^{(\alpha)}\}] + \sum_{\alpha} \langle \delta v \rangle_{WS} (\bar{n}_{\alpha}) \int d\vec{r} \Theta^{(\alpha)}(\vec{r}) [n(\vec{r}) - n_+^{(\alpha)}(\vec{r})] \\ + \sum_{\alpha} [\bar{w}_R(\bar{n}_{\alpha}) + \varepsilon_M(\bar{n}_{\alpha})] \int d\vec{r} n_+^{(\alpha)}(\vec{r})$$

α enumerates different regions

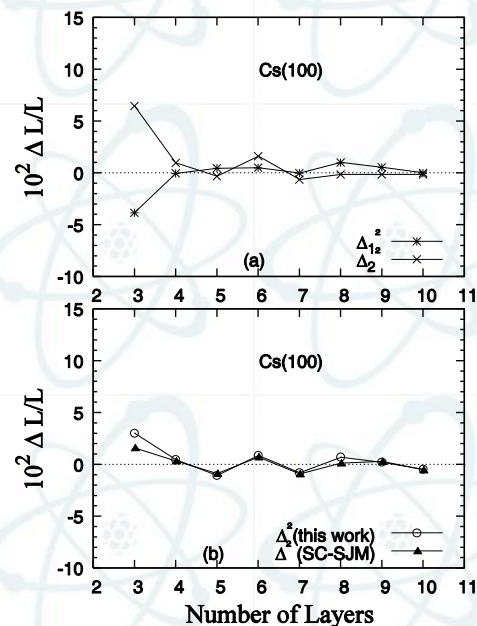
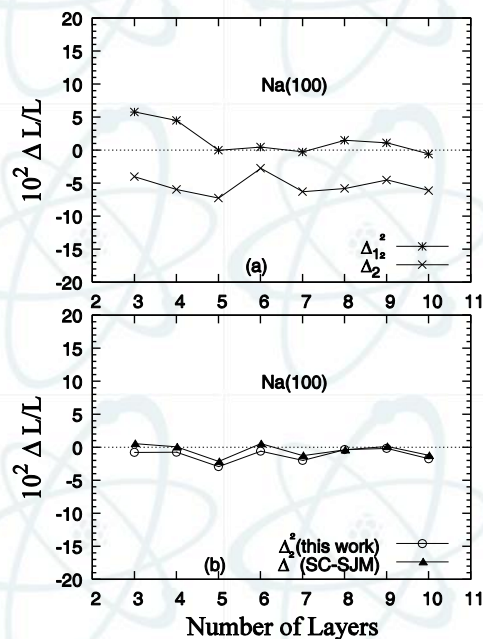
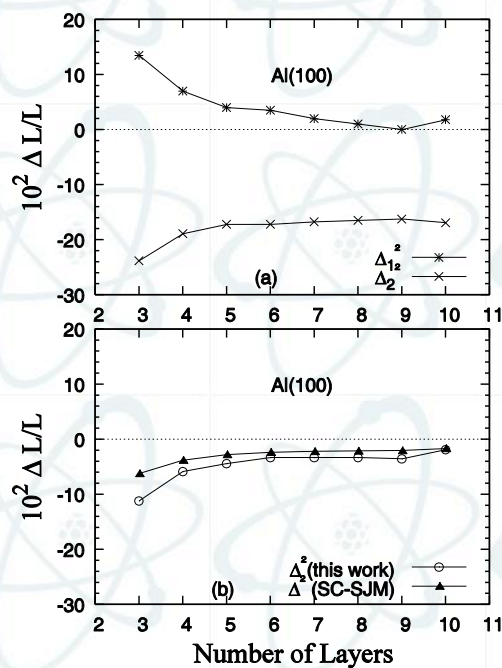
M. Payami, T. Mahmoodi, *Can. J. Phys.* **89**, 967 (2011)

Calculation Method

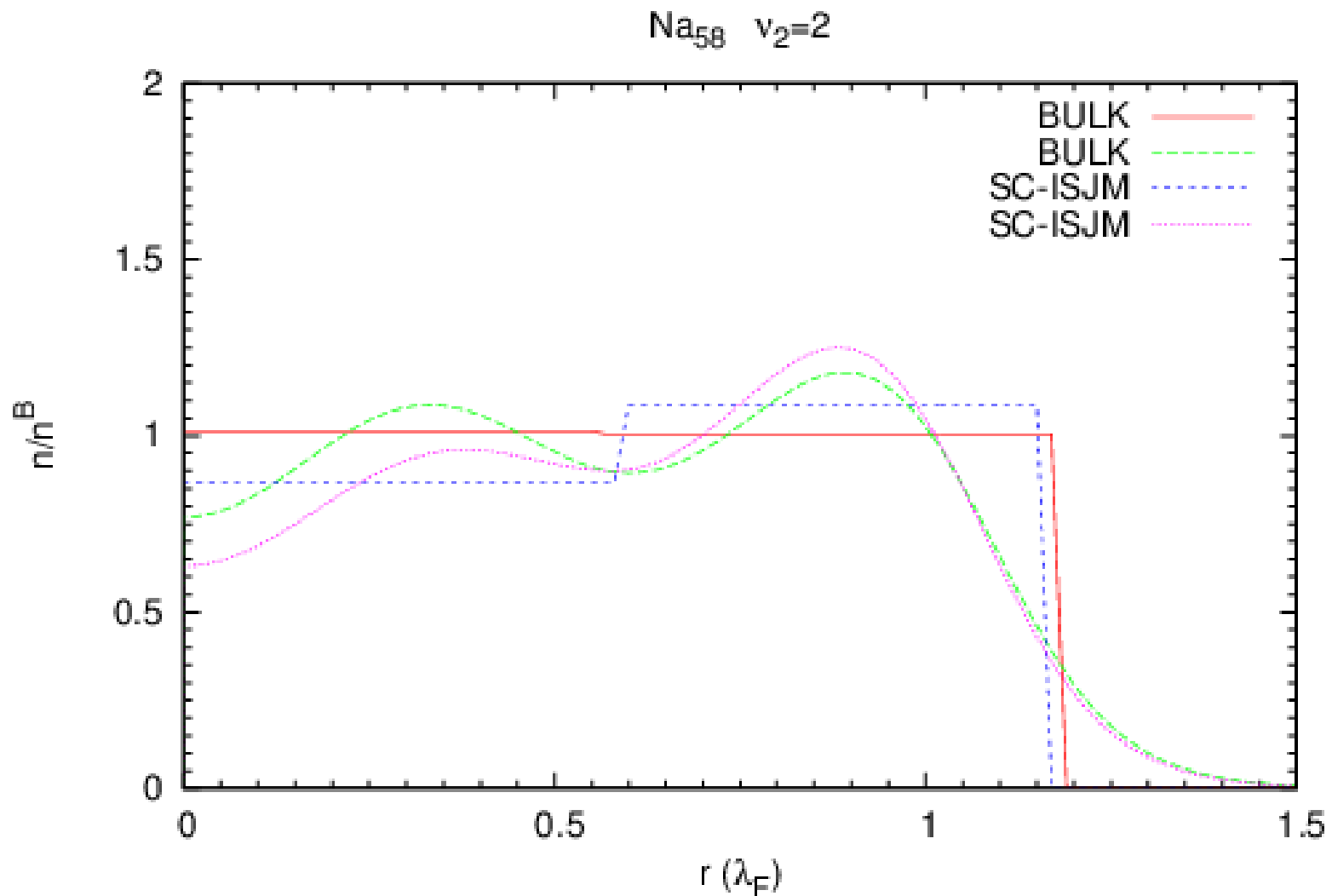
Equilibrium State:

$$E_0 / N \equiv E(\{\bar{n}_\alpha^\dagger\}) / N = \min_{\{\bar{n}_\alpha\}} E(\{\bar{n}_\alpha\}) / N$$

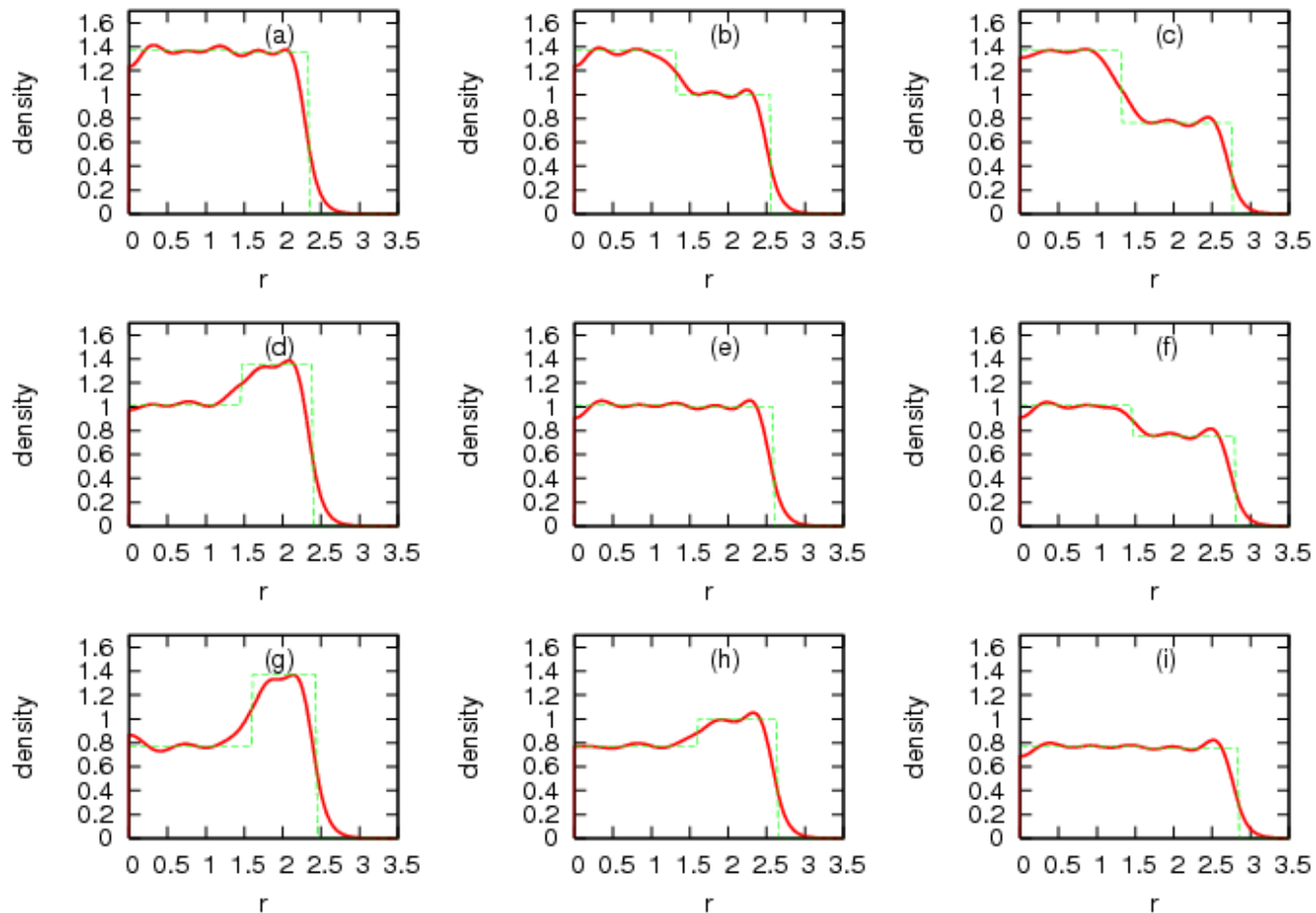
SC-ISJM Results for Thin films



SC-ISJM results fo metal clusters

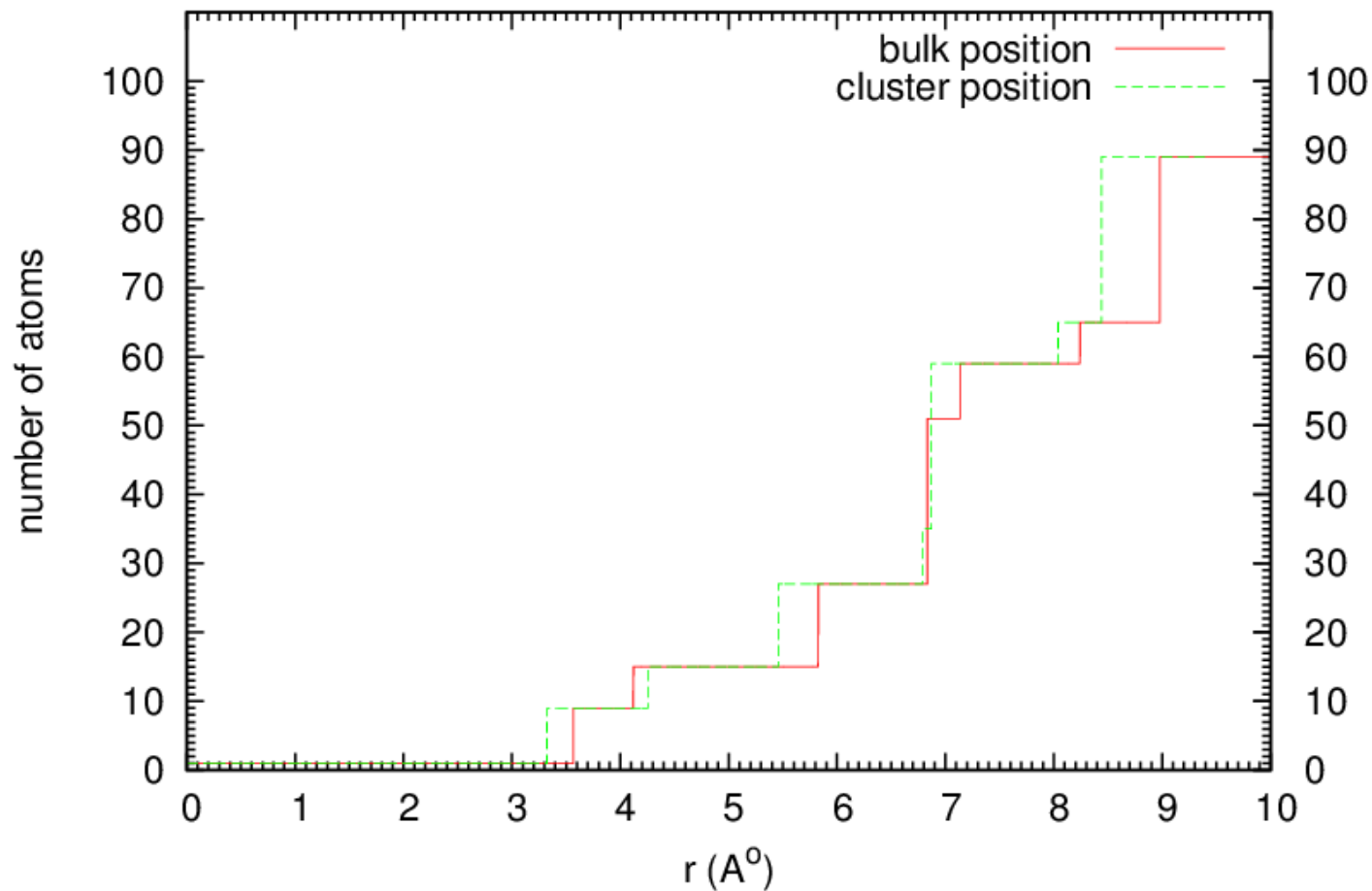


$Al^{204}, n_2=2$



Results: First-Principles

Na₈₉



از توجه شما بینهایت سیاسگزارم

Our Group



M. Payami

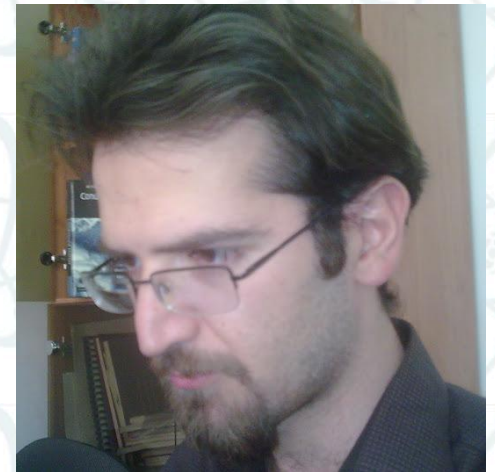


Dr. T. Mahmoodi



Dr. N. Zare

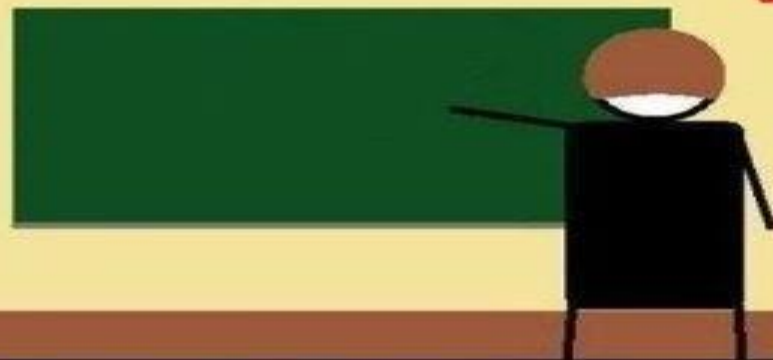
نوزدهمین کنفرانس بهار فیزیک
۲۷-۲۸ اردیبهشت ۱۳۹۱ پژوهشگاه دانشهای بنیادی



Y. Taghipour Azar
PhD Student

چیزی که دانشجو یادش میمونه

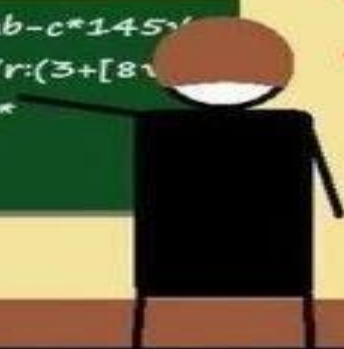
4



نوشته های روی تخته !

1

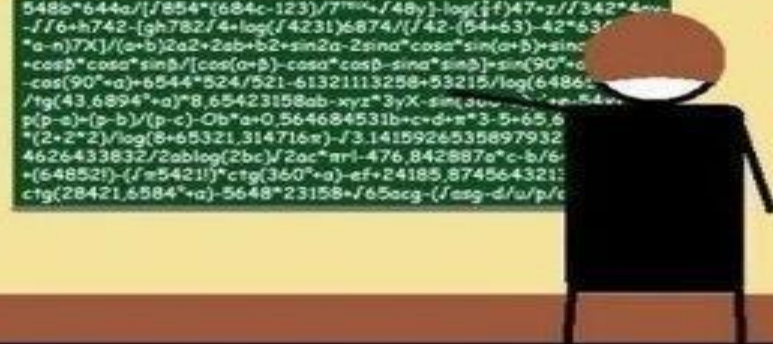
$12\sqrt{6*7}:(6+2\sqrt{4})*2+ab-c*145\sqrt{6}$
 $1+-5x+6y*22\sqrt{4d}+2\sqrt{r}:(3+[8\sqrt{d}+2\sqrt{r}]:3+2\sqrt{v})*34\sqrt{4u}*3ea*$



چیزی که تو امتحان میاد !؟

5

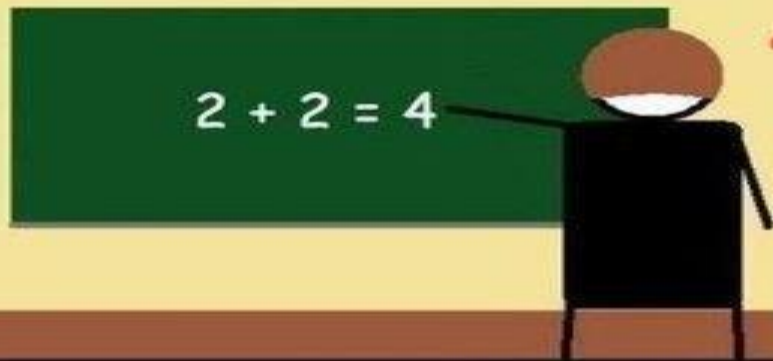
$548b^*644a/[f854*(684c-123)/7^{**}/48y]-\log([f]47*x/f342*4n-$
 $-f6+h742-[gh782/4+\log(f4231)6874/(f42-(54+63)-42*63$
 $*a-n)7X]/(a-b)2a2+2ab+b2+\sin2a-2\sin a*\cos a*\sin(a+b)+\sin$
 $+ \cos b*\cos a*\sin b/[\cos(a+b)-\cos a*\cos b-\sin a*\sin b]-\sin(90^*+a$
 $-\cos(90^*+a)+6544*524/521-61321113258+53215/\log(6486$
 $/tg(43.6894^*+a)*8.65423158ab-xyz*3yX-\sin a$
 $p(p-a)=(p-b)/(p-c)-Ob^*a+0.564684531b+c+d*\pi^3-5+65.6$
 $*(2+2^2)/\log(8+65321.314716\pi)-/3.1415926535897932$
 $4626433832/2ab\log(2bc)/2ac*\pi-476.842887e^*c-b/6$
 $+(648521)-(f=54211)*ctg(360^*+a)-ef+24185.874564321:$
 $ctg(28421.6584^*+a)-5648*23158+/65ocg-(fscg-d/a/p/c$



توضیح استاد !؟

2

$2 + 2 = 4$



مشاهدات نظافتکار !

6



چیزی که دانشجو میبینه :دی

3

而不是鍵入一個美好的譯員
 胡說我有一個夢想. 夢想難E
 話'的事情在衣櫃裡. 他媽的始
 備到有經驗的獵人阿哈小好

