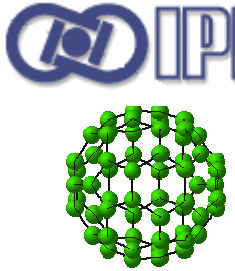

Department of
Nano-Science

Advanced School of Recent Progress in
Condensed Matter Physics and
Strongly Correlated Systems

School of Physics, IPM

(Institute for Studies in Theoretical Physics and Mathematics)

July 5 – 9, 2008

Tehran, IRAN

جوابهای خودسازگار ساختار الکترونی $PrBa_2Cu_3O_7$

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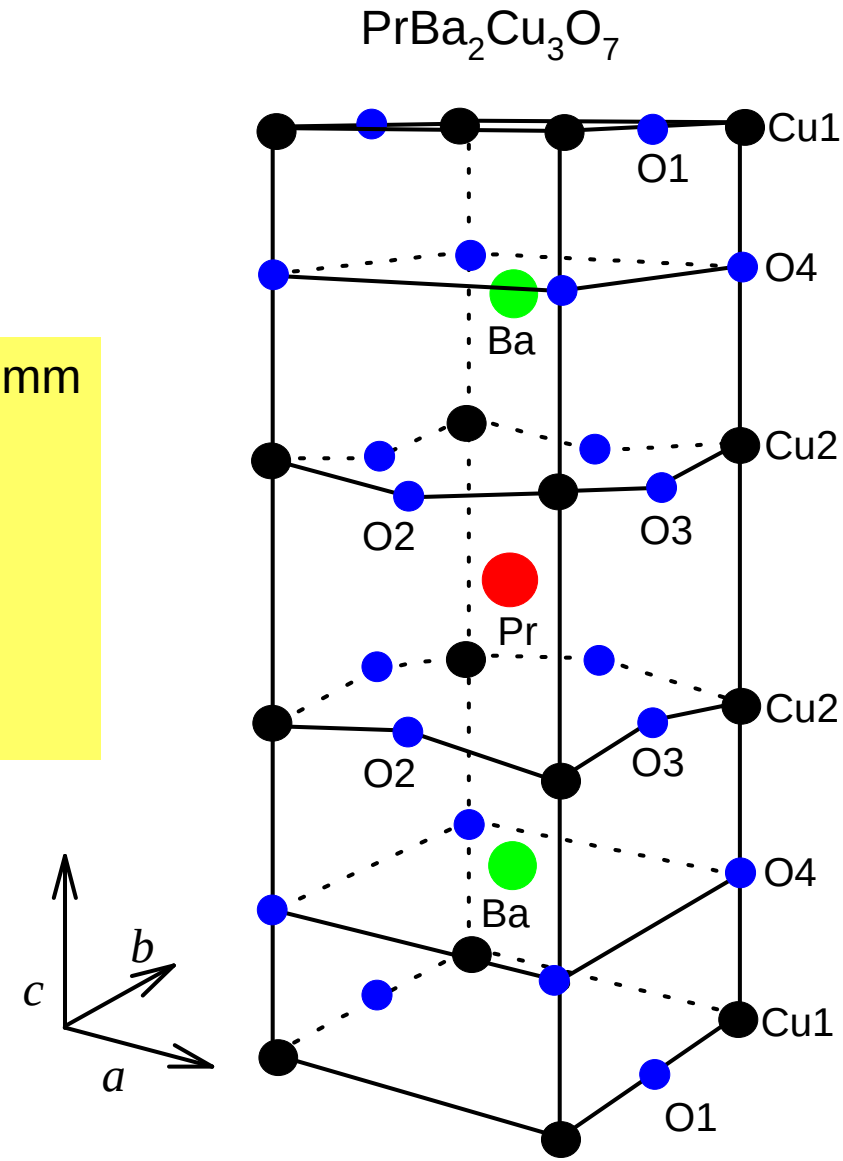
۱ آزمایشگاه پژوهشی ابررسانایی، دانشکده فیزیک دانشگاه تهران

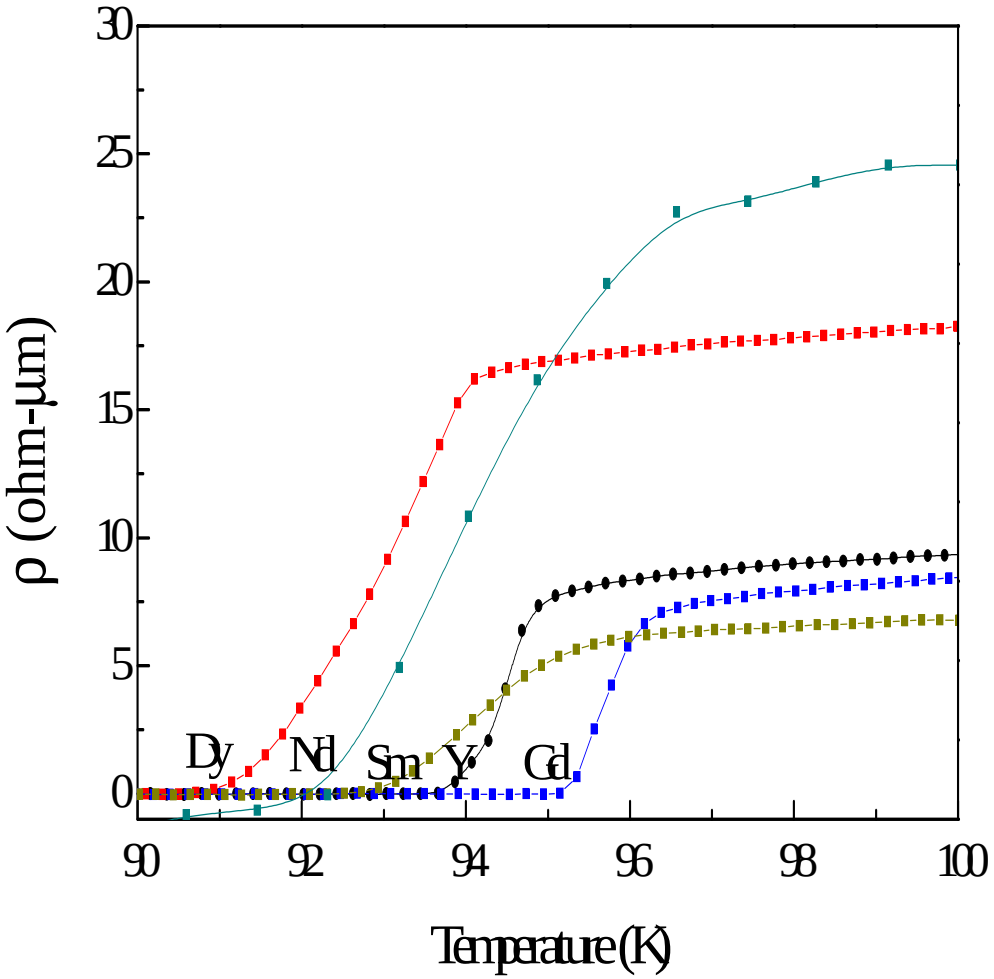
۲ پژوهشکده علوم نانو، IPM

Orthorhombic P4/mmm

a=3.83 Å
b=3.88 Å
c=11.68 Å

13 atoms/cell

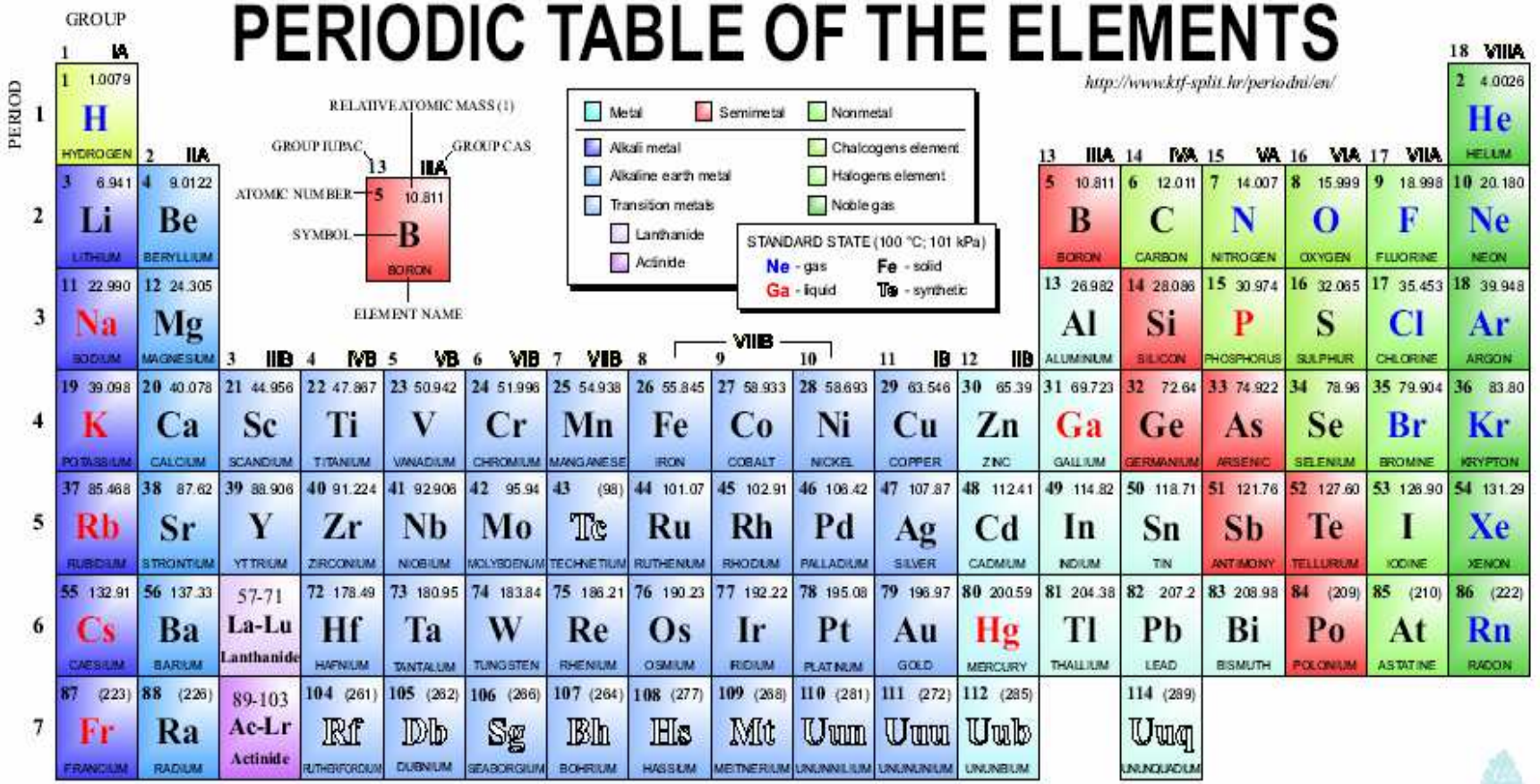




- $RBa_2Cu_3O_{7-\delta}$ (R-123)
- Gd - : 95.8 K
- Y- : 94.2 K
- Sm- : 93.2 K
- Nd- : 92.2 K
- Dy- : 91.8 K

PERIODIC TABLE OF THE ELEMENTS

http://www.ktf-split.hr/periodni/en/



(1) Pure Appl. Chem., **73**, No. 4, 667-683 (2001)

Relative atomic mass is shown with five significant figures. For elements have no stable nuclides, the value enclosed in brackets indicates the mass number of the longest-lived isotope of the element.

However three such elements (Th, Pa, and U) do have a characteristic terrestrial isotopic composition, and for these an atomic weight is tabulated.

Editor: Aditya Vardhan (adivar@netlinx.com)

$[Xe]4f^{3}6S^{2}]$

Pr

Orthorhombic $PrBa_2Cu_3O_{7-\delta}$

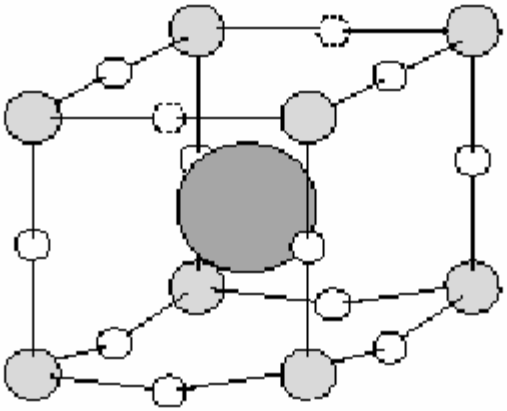
- Name: praseodymium
- Symbol: Pr
- Atomic number: 59
- Atomic weight: 140.90765 (2)

Justifying the insulator behavior of $PrBa_2Cu_3O_{7-\delta}$

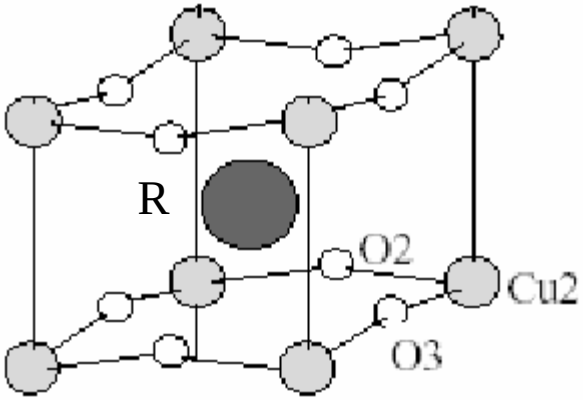
Hole filling:	Horn et al., Phys. Rev. B 36 (1987) 3895.
Pair breaking:	Peng et al., Phys. Rev. B 40 (1989) 4517.
Hybridyzation (FR):	Fehrenbacher & Rice, Phys. Rev. Lett. 70 (1993) 3471.
Charge transfer:	Khomskii, J. Supercond. 6 (1993) 69.
Hybridyzation:	Wang et al., Phys. Rev. B 50 (1994) 10350.
LM:	Liechtenstein & Mazin, Phys. Rev. Lett. 74 (1995) 1000.
Mis-substitution:	Blackstead & Dow, Phys. Rev. B 57 (1995) 11830.
Semiconductor model:	Kakinuma et al., Phys. Rev. B 56 (1997) 3494.
Percolation:	Horii et al., Physica C 282 (1997) 809.
Coexistence:	Yu et al., Phys. Rev. B 59 (1999) 3845.

Superconducting $PrBa_2Cu_3O_{7-\delta}$!!!

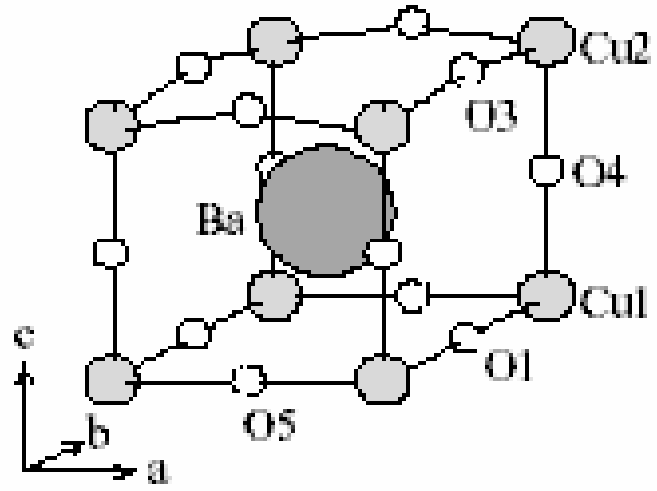
1) Zou et al., Phys. Rev. Lett. 50 (1998) 1074.	single crystal
2) Blackstead & Dow, , Phys. Rev. B 57 (1995) 11830.	powders, thin films
3) Luszczek et al., Physica C 322 (1999) 57.	single crystal
4) Usagawa et al., JJAP 36 (1997) L1583.	thin film
5) Shukla et al., Phys. Rev. B 59 (1999) 12127.	single crystal
6) Araujo-Moreira et al., Physica B 284-288 (2000) 1033.	polycrystal



$BaCuO_3$



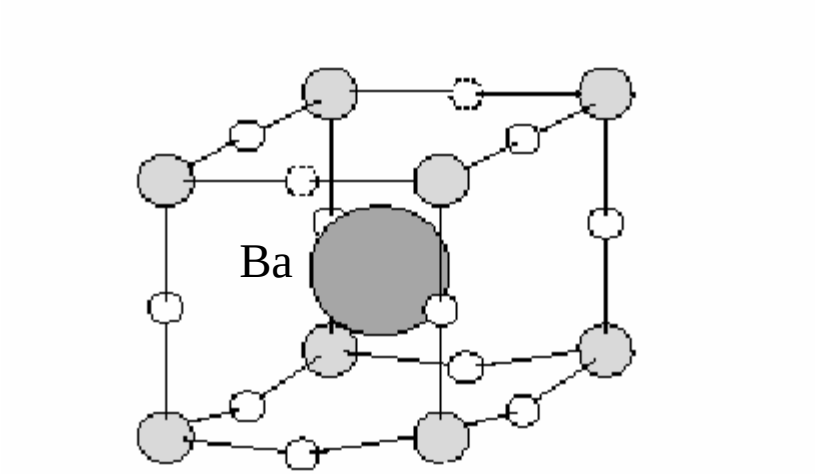
$PrCuO_2$



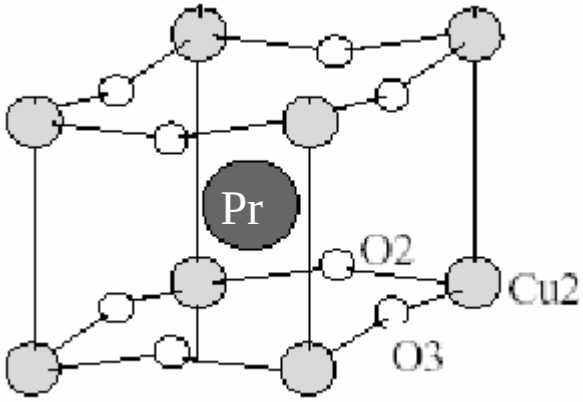
$BaCuO_3$

- Equivalent positions
- Small ξ

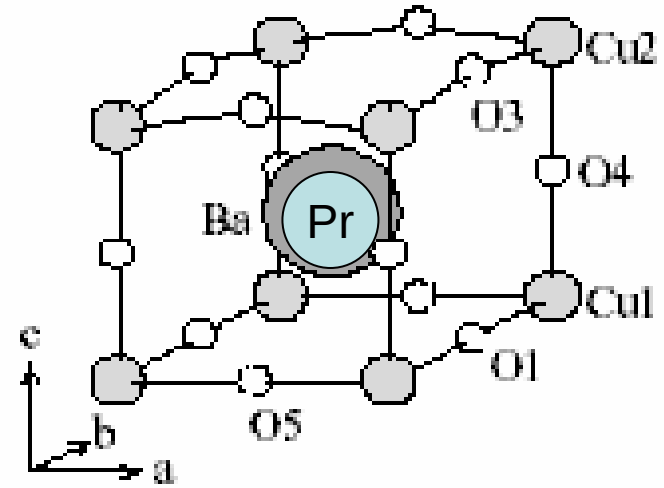
Mis-substitution



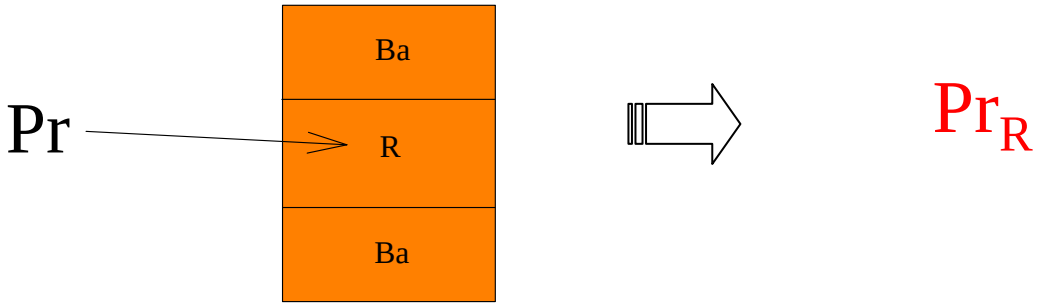
$BaCuO_3$



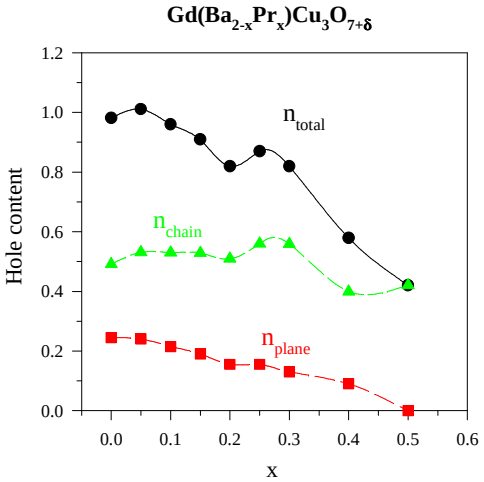
$RCuO_2$

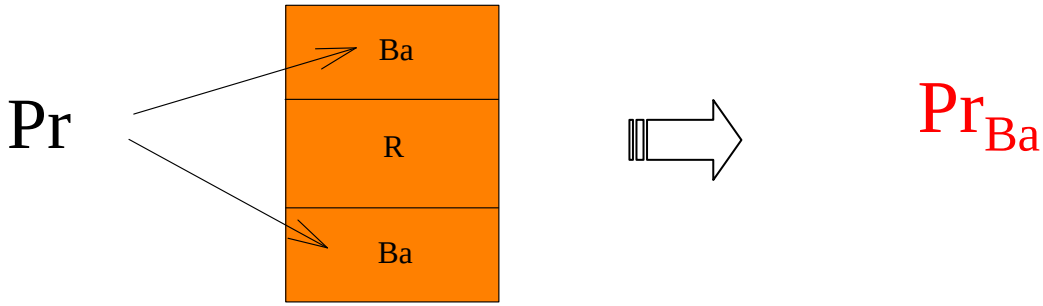


$BaCuO_3$



- M.R. Mohammadizadeh and M. Akhavan,, Eur. Phys. J. B 33 (2003) 381-390.
- M.R. Mohammadizadeh, H. Khosroabadi, and M. Akhavan, Physica B, 321 (2002) 301-304.





- *M.R. Mohammadizadeh and M. Akhavan, Phys. Rev. B 68 (2003) 104516.*

Computational details

(L/APW+lo) ➔ WIEN2k DFT

Exchange-correlation energy ➔ LSDA & LSDA+U

Rotational invariant LSDA+U ➔ around mean field (AMF) version

U & J ➔ EFG

Ferromagnetic ordering

8×8×2 mesh (200 special *k*-points) ➔ (16 *k*-points 1BZ)

Plane wave cutoff of $K_{max} = 7.5/R_{MT}$

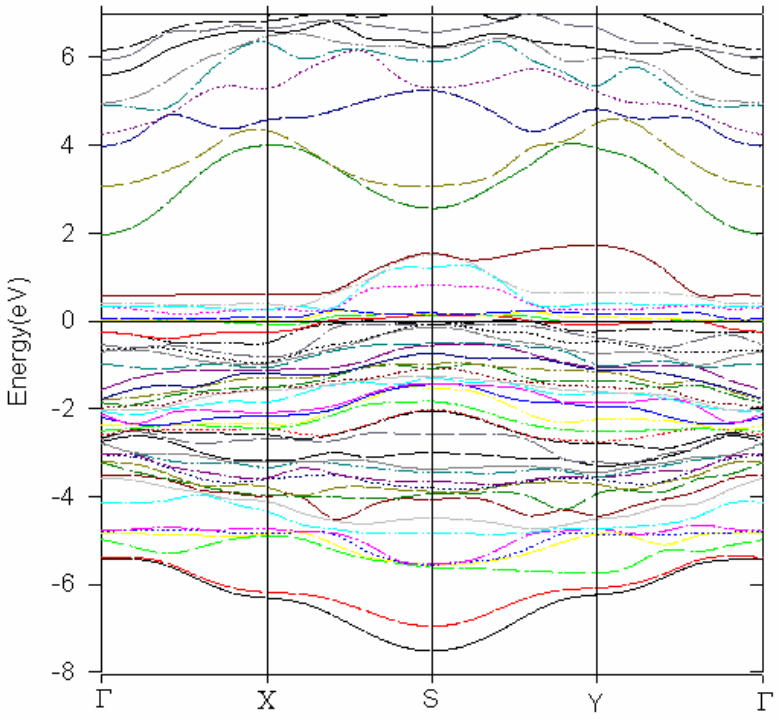
Charge density ➔ $G_{max} = 14$

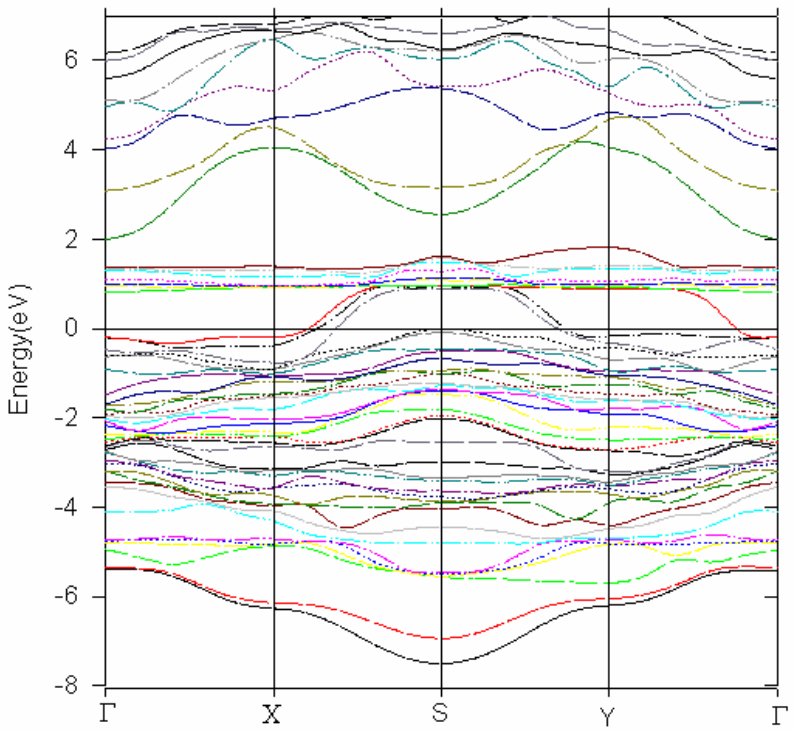
R_{MT} of Pr, Y, Ba, Cu, and O atoms / 2.8, 2.74, 2.9, 1.8, 0.65 B_{ohr}

Total energy ➔ 0.1 meV/Cell

$PrBa_2Cu_3O_7$

LSDA





- Pr-4f , LSDA ➔ LSDA+U
- splitting ➔ Magnetic moment

LSDA+U

- ایده پشت آن، همان ایده های ساخت هامیلتونی های مدل است .
- جملاتی شبیه $\frac{1}{2}U\sum_i n_{i\uparrow}n_{i\downarrow}$ در ها میلتونی هابارد و اندرسون
- منحصر به فرد نیست.
- از روی GW هم می توان ...

دستگاه N الکتروني با بر همکنش کولني

$$W = \frac{1}{2}\sum_{i\neq j}^{N} V_{ee}(i,j)$$

$$V_{ee}(i,j) = \frac{1}{4\pi\varepsilon_0}\frac{1}{|\vec{r}_i - \vec{r}_i|}$$

$$\Psi(\vec{r}_1, s_1, \cdots, \vec{r}_N, s_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_1(\vec{r}_1, s_1) & \cdots & \psi_1(\vec{r}_N, s_N) \\ \vdots & & \vdots \\ \psi_N(\vec{r}_1, s_1) & \cdots & \psi_N(\vec{r}_N, s_N) \end{vmatrix}$$

$$\langle \Psi | W | \Psi \rangle = \frac{1}{2}\sum_{ij=1}^{N} \langle ij | ij \rangle - \frac{1}{2}\sum_{ij=1}^{N} \langle ij | ji \rangle$$

Direct Exchange

LSDA+U

یک جمله براي هر اتم با پوسته نیمه پر d و f به انرژي تبادلي- همبستگي
تقریب LSDA اضافه

$$E_U = \langle \Psi | W | \Psi \rangle_l - E_{dc}$$

SIC

AMF

FLL+AMF

Self-Interaction Correction

$$E_{dc} = \frac{1}{2} UN(N-1) - \frac{1}{2} J\left[N\uparrow\left(N\uparrow -1\right) + N\downarrow\left(N\downarrow -1\right)\right]$$

$$E_{dc} = UN_\uparrow N_\downarrow + \frac{1}{2}\left(N_\uparrow^2 + N_\downarrow^2\right)\frac{2l}{2l+1}\left(U - J\right)$$

Around the Mean Field

$$N_\sigma = \sum_{m=-l}^{l} n_{mm}^{\sigma\sigma} = Tr\left(n_{mm'}^{\sigma\sigma}\right) = (2l+1)\left\langle n^\sigma \right\rangle$$

$$N = N_\uparrow + N_\downarrow$$

$$U = \frac{1}{(2l+1)^2}\sum_{mm'} U_{mm'}$$

پارامتر هابارد

$$J = U - \frac{1}{2l(2l+1)}\sum_{mm'}\left(U_{mm'} - J_{mm'}\right)$$

پارامتر تبادلي

$$U_{mm'} = \left\langle mm' \middle| V_{ee} \middle| mm' \right\rangle$$

$$J_{mm'} = \left\langle mm \middle| V_{ee} \middle| m'm' \right\rangle$$

روشهای مشخص کردن مقادیر U و J

- سعی و خطا وجود کمیت تجربی!

سازگاری همه کمیتها ی تجربی!

- تجربی (XPS)

- ابتدا به ساکن ⟵ تطابق با آزمایش

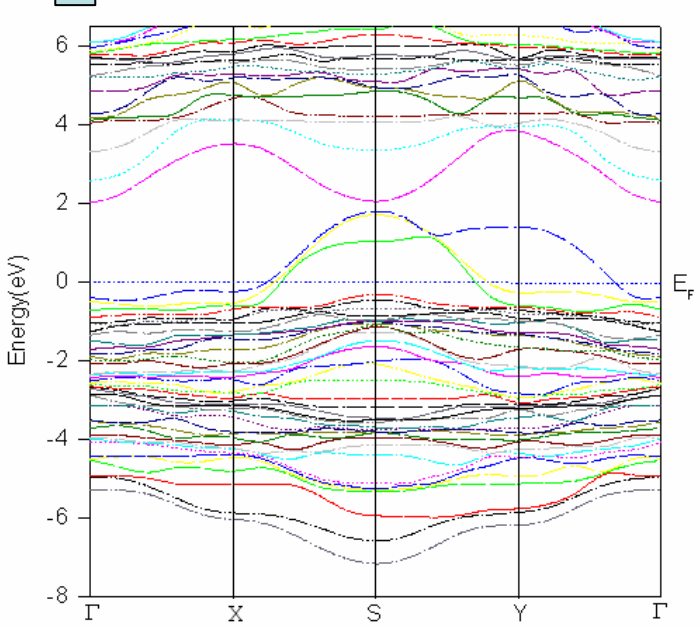
مشکلات LSDA+U

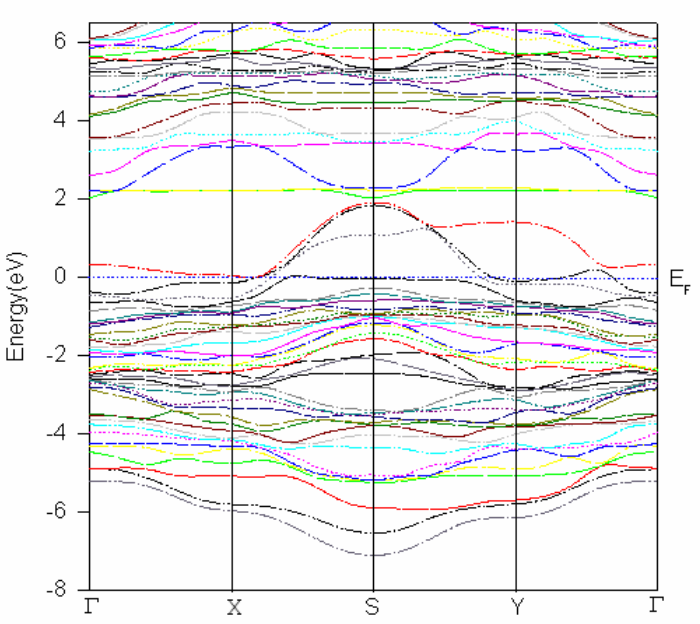
- وابسته بودن روش به مقدار U و J
- ابرسلول ⟵ حجم زیاد محاسبات
- مدل: وابسته به نسخه (SIC-AMF-...)
- گاهی پایه اثر گذار است:

  LMTO

  LAPW ⟵ U های متفاوت
- ماتریس عدد اشغال متفاوت ⟵ جواب متفاوت

$Pr(BaPr)Cu_3O_7$ LSDA+U(Pr)

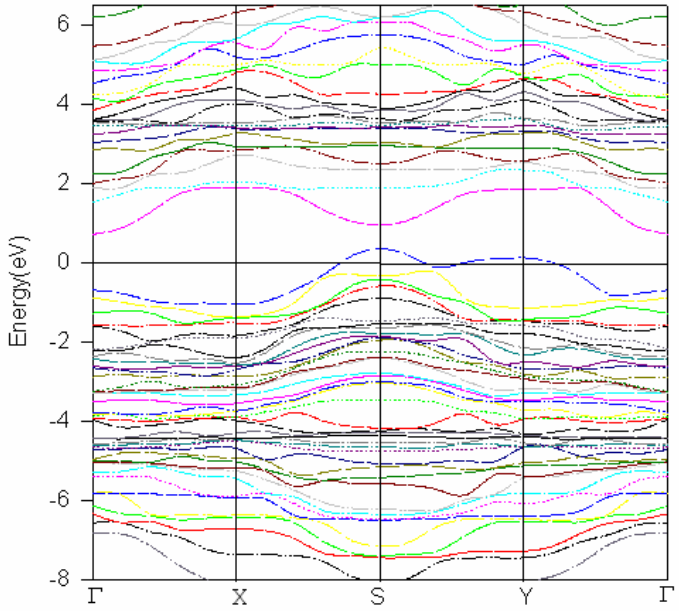


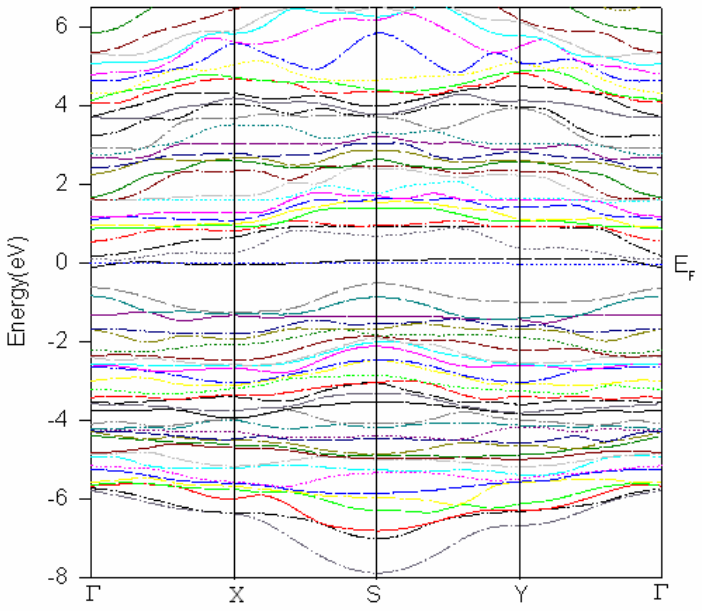


- metal
- $hole_{Cu\text{-}O}$ ➔ decreases

$Pr(BaPr)Cu_3O_7$

LSDA+U(Pr,Cu)





- approaching to insulator
- U & J, ion relax, cell relax, O,

EFG

The calculated EFG (Vzz) in units of 10^{21} Vm^{-2} at oxygen and copper sites of PrBa2Cu3O7 for various sets of U and J values in Ry.

case	J_{Pr}	U_{Pr}	J_{Cu1}	U_{Cu1}	J_{Cu2}	U_{Cu2}	Cu1	Cu2	O1	O2	O3	O4
1	0	0	0	0	0	0	5.9	-3	17.6	9.7	9.9	12
2	0	0.3	0	0	0	0	6.2	-5.2	17.9	12.7	12	12.1
3	0	0.5	0	0	0	0	6.3	-5.3	18	13.4	13.8	12.2
4	0	0.74	0	0	0	0	6.3	-5.3	17.9	13.4	13.3	12.2
5	0.05	0.74	0.1	0.25	0.1	0.25	6.3	-6.2	18.1	12.8	13.9	12.2
6	0.05	0.74	0.1	0.35	0.1	0.35	7.6	-10.7	17.4	12	12.7	11.8
7	0.05	0.74	0.1	0.55	0.1	0.55	-10.6	-16.6	17.1	10.2	10.9	11.4
8	0.05	0.74	0.1	0.75	0.1	0.75	-13.4	-20.3	15.5	9.5	10	10.2
9	0	0	0.1	0.45	0.1	0.45	7.9	-11.2	16.1	7.8	8.0	11.7
10	0.05	0.54	0.1	0.45	0.1	0.45	9.0	-14.9	17.8	10.7	10.8	12.1
11	0.05	0.74	0	0	0.1	0.55	6.4	-16.6	18.8	9.9	10.5	11.6
12	0.05	0.74	0.1	0.45	0.1	0.25	8.8	-6.2	17.1	12.5	13.2	12.1

η

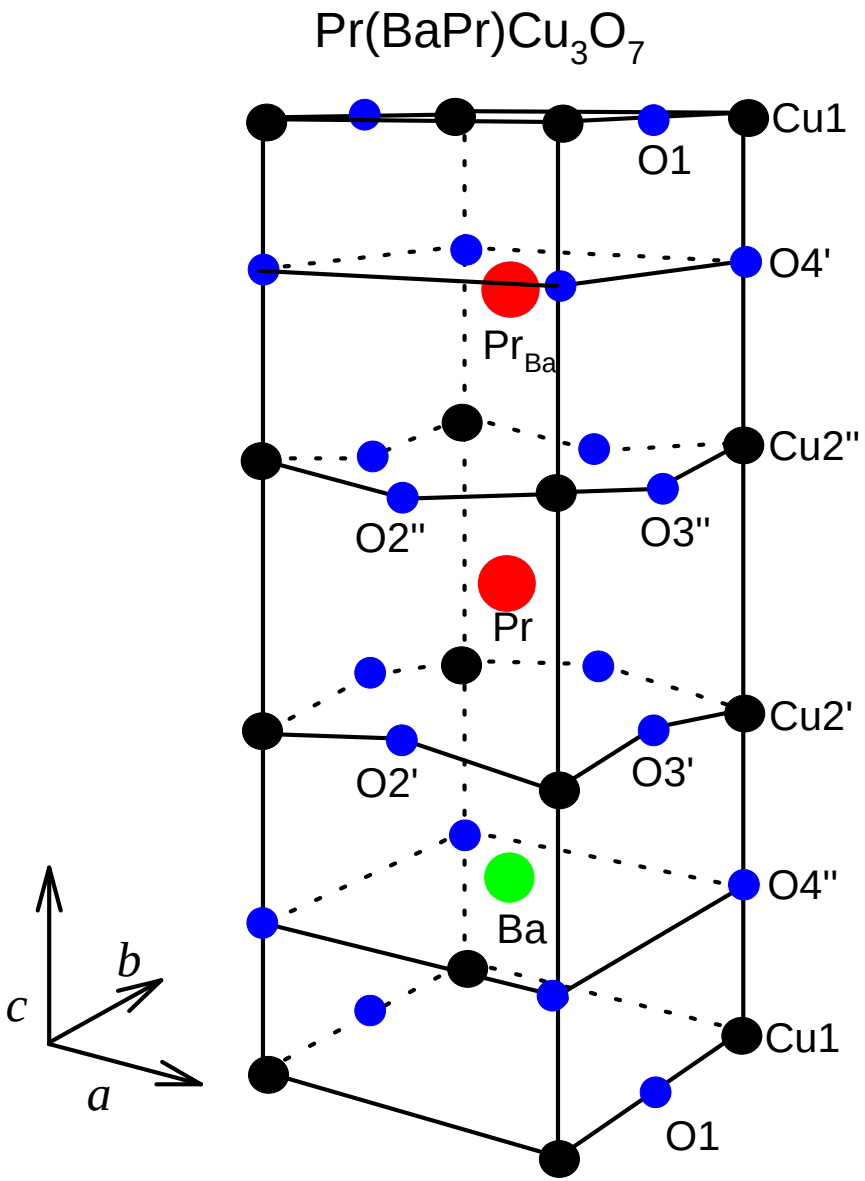
The calculated asymmetry parameter η at oxygen and copper sites of $PrBa_2Cu_3O_7$ for various sets of U and J values in Ry.

case	J_{Pr}	U_{Pr}	J_{Cu1}	U_{Cu1}	J_{Cu1}	U_{Cu2}	Cu1	Cu2	O1	O2	O3	O4
1	0	0	0	0	0	0	0.4	0.1	0.4	0.1	0.1	0.3
2	0	0.3	0	0	0	0	0.5	0.1	0.4	0.3	0.1	0.3
3	0	0.5	0	0	0	0	0.5	0.1	0.3	0.3	0.2	0.2
4	0	0.74	0	0	0	0	0.5	0.1	0.3	0.2	0.2	0.2
5	0.05	0.74	0.1	0.25	0.1	0.25	0.3	0.0	0.3	0.3	0.3	0.2
6	0.05	0.74	0.1	0.35	0.1	0.35	0.7	0.0	0.4	0.3	0.2	0.2
7	0.05	0.74	0.1	0.55	0.1	0.55	0.9	0.0	0.5	0.4	0.3	0.3
8	0.05	0.74	0.1	0.75	0.1	0.75	0.7	0.1	0.5	0.4	0.4	0.3
9	0	0	0.1	0.45	0.1	0.45	1.0	0.0	0.5	0.2	0.2	0.4
10	0.05	0.54	0.1	0.45	0.1	0.45	0.9	0.0	0.4	0.3	0.3	0.3
11	0.05	0.74	0	0	0.1	0.55	0.6	0.0	0.4	0.4	0.3	0.2
12	0.05	0.74	0.1	0.45	0.1	0.25	0.9	0.1	0.4	0.3	0.2	0.3

EFG	O1	O2	O3	O4
First calculation	17.8	12.7	12.9	12.1
Second calculation	17.7	13.1	13.3	12.2
Experiment: nonsuperconducting Pr123 sample [29]	---	6.9	10.2	11.1
Experiment: superconducting Y123 sample [36]	17.3	10.5	10.2	11.6

The experimental EFG (Vzz) in units of 10^{21} Vm^{-2} and asymmetry parameter η at oxygen sites of nonsuperconducting $PrBa_2Cu_3O_{7-\delta}$, $YBa_2Cu_3O_{7-\delta}$, and $YBa_2Cu_3O_{6.6}$.

		O1	O2	O3	O4
$PrBa_2Cu_3O_{7-\delta}$ [46]	EFG	---	6.9	10.2	11.1
	η	---	0.09	0.40	0.24
$YBa_2Cu_3O_{7-\delta}$ [24]	EFG	17.3	10.5	10.2	11.6
	η	0.41	0.21	0.24	0.32
$YBa_2Cu_3O_{6.6}$ [51]	EFG	---	9.4	9.4	11.0
	η	---	0.23	0.23	0.29


Pr(BaPr)Cu3O7
Cu1
O1
O4'
PrBa
Cu2"
O2"
O3"
Pr
Cu2'
O2'
O3'
O4"
Ba
Cu1
O1
b
c
a

The calculated EFG (Vzz) in units of 10^{21} Vm^{-2} and asymmetry parameter η at O2 and O3 sites of $Pr(BaPr)Cu_3O_7$ in LSDA

	O2′	O3′	O2″	O3″
EFG	5.9	6.0	5.0	4.9
η	0.2	0.2	0.3	0.3

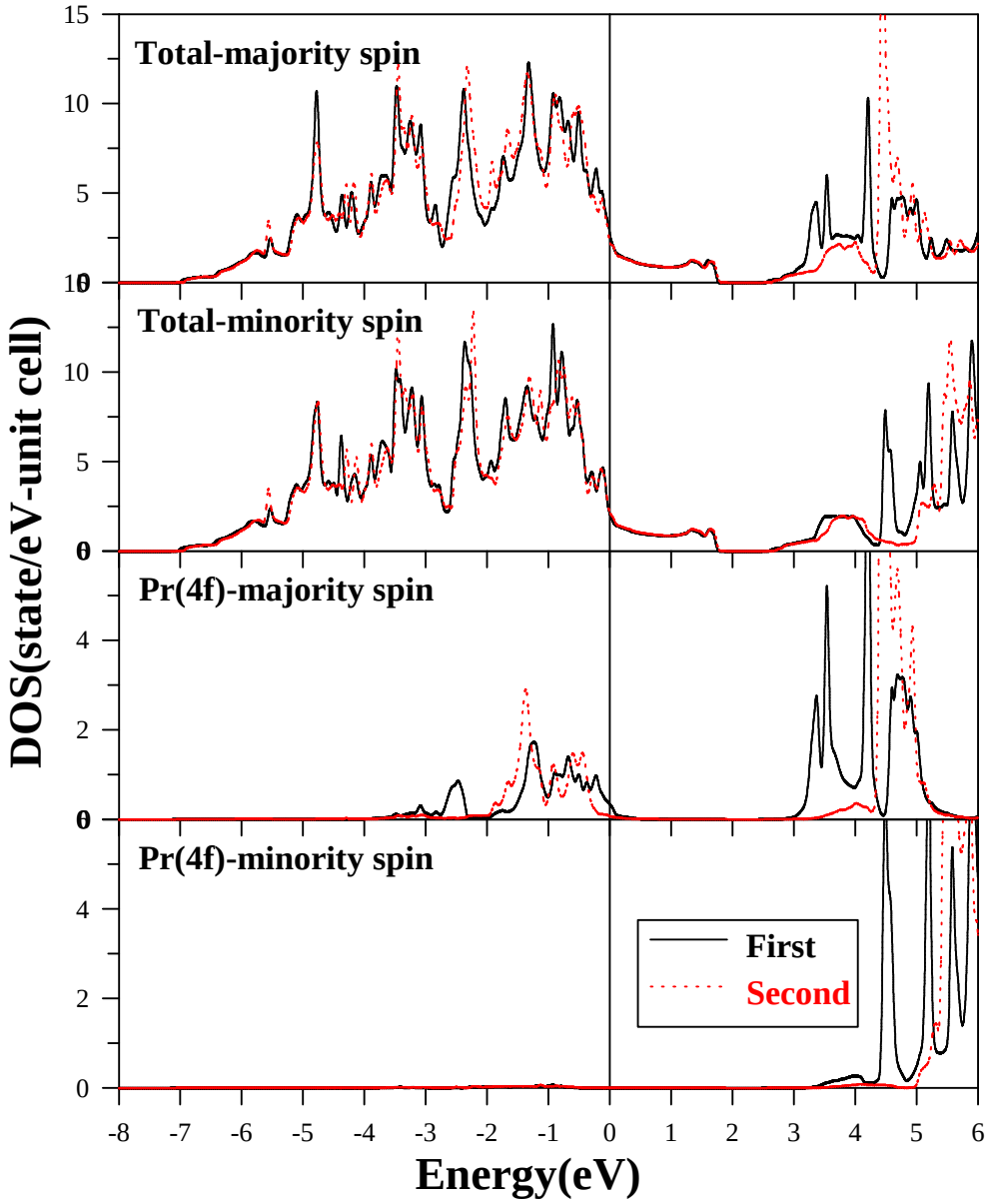
V. Ghanbarian , M.R. Mohammadizadeh, Phys. Stat. Sol. c 3 (2006) 3122.
V. Ghanbarian , M.R. Mohammadizadeh, Euro. Phys. J. B 61 (2008) 309.

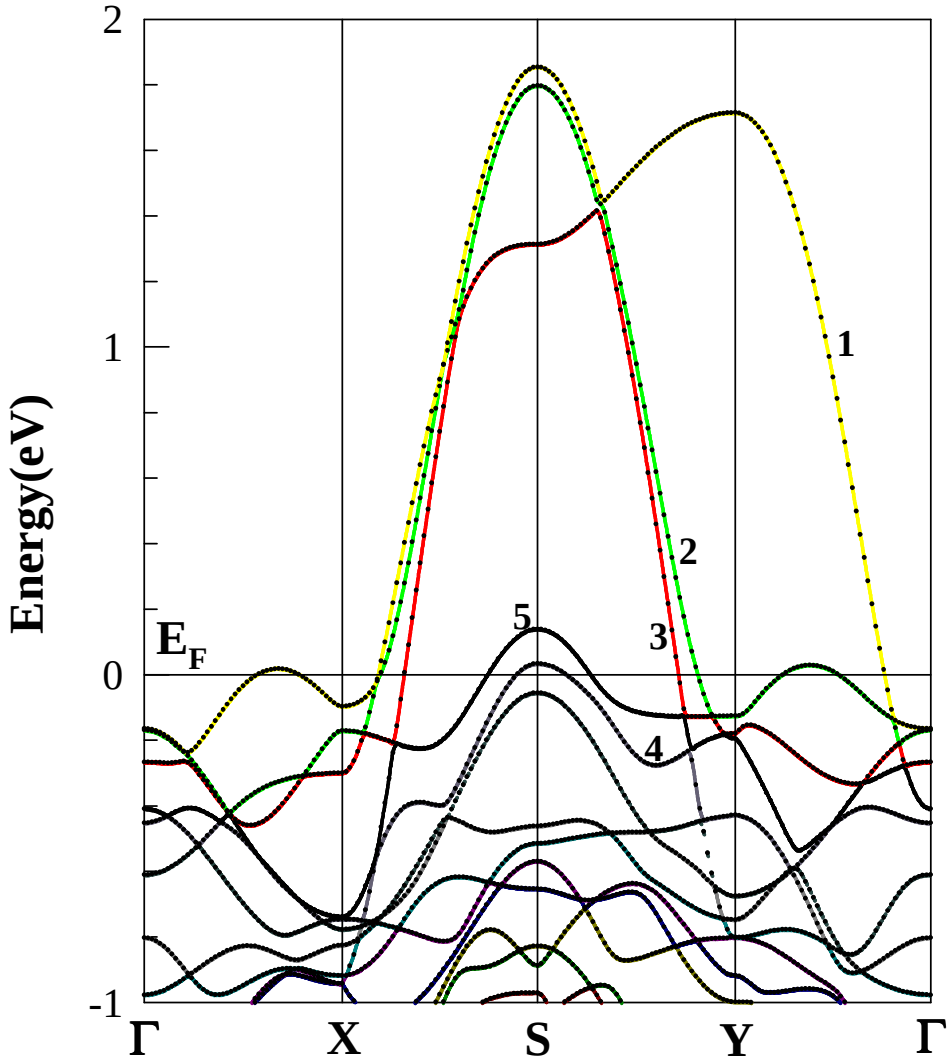
The EFG (Vzz) in units of 10^{21} Vm^{-2} at oxygen and copper sites of $PrBa_2Cu_3O_7$

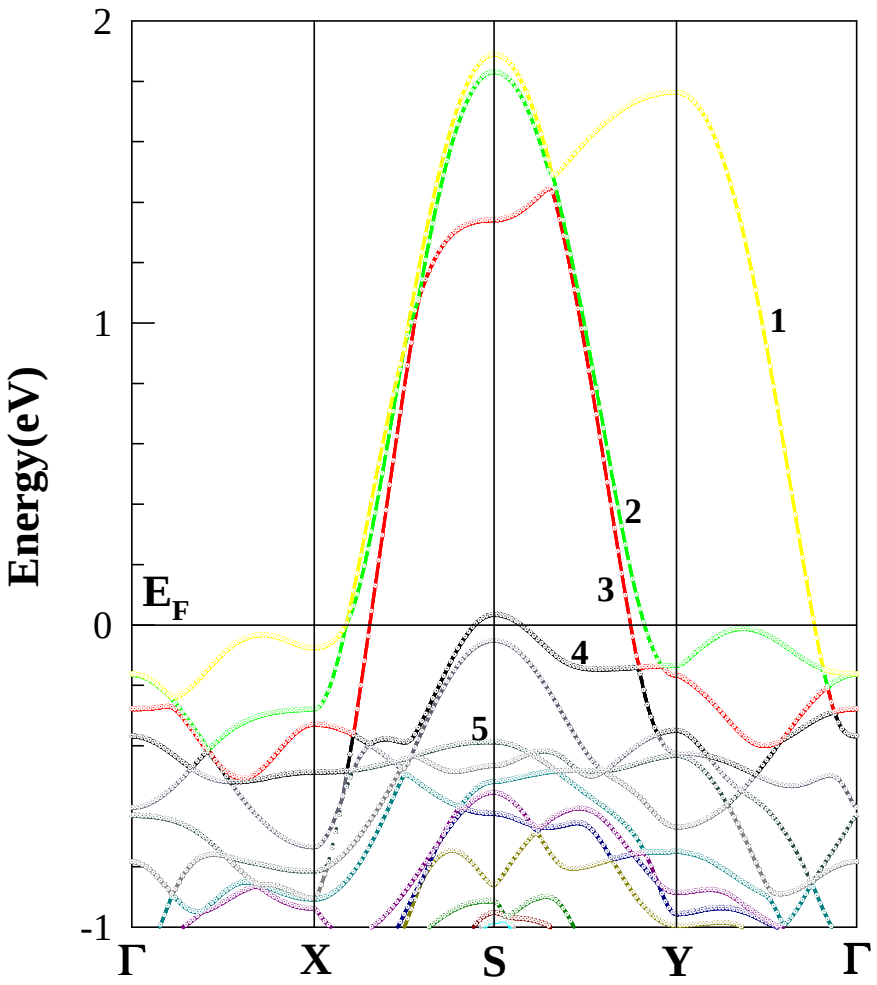
case	Cu1	Cu2	O1	O2	O3	O4
4+	6.1	0.6	17.2	8.3	8.3	11.6
itinerant	6.5	-2.5	17.8	9.4	9.8	12.0
3+	7.0	-5.6	17.8	13.1	13.7	11.7

Asymmetry parameter (η) at oxygen and copper sites of PrBa2Cu3O7

case	Cu1	Cu2	O1	O2	O3	O4
4+	0.6	0.3	0.3	0.2	0.3	0.2
itinerant	0.6	0.2	0.4	0.2	0.2	0.2
3+	0.7	0.1	0.3	0.3	0.3	0.1


Total-majority spin
Total-minority spin
Pr(4f)-majority spin
Pr(4f)-minority spin
First
Second
DOS(state/eV-unit cell)
Energy(eV)
15
10
5
0
10
5
0
4
2
0
4
2
0
-8
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
4
5
6

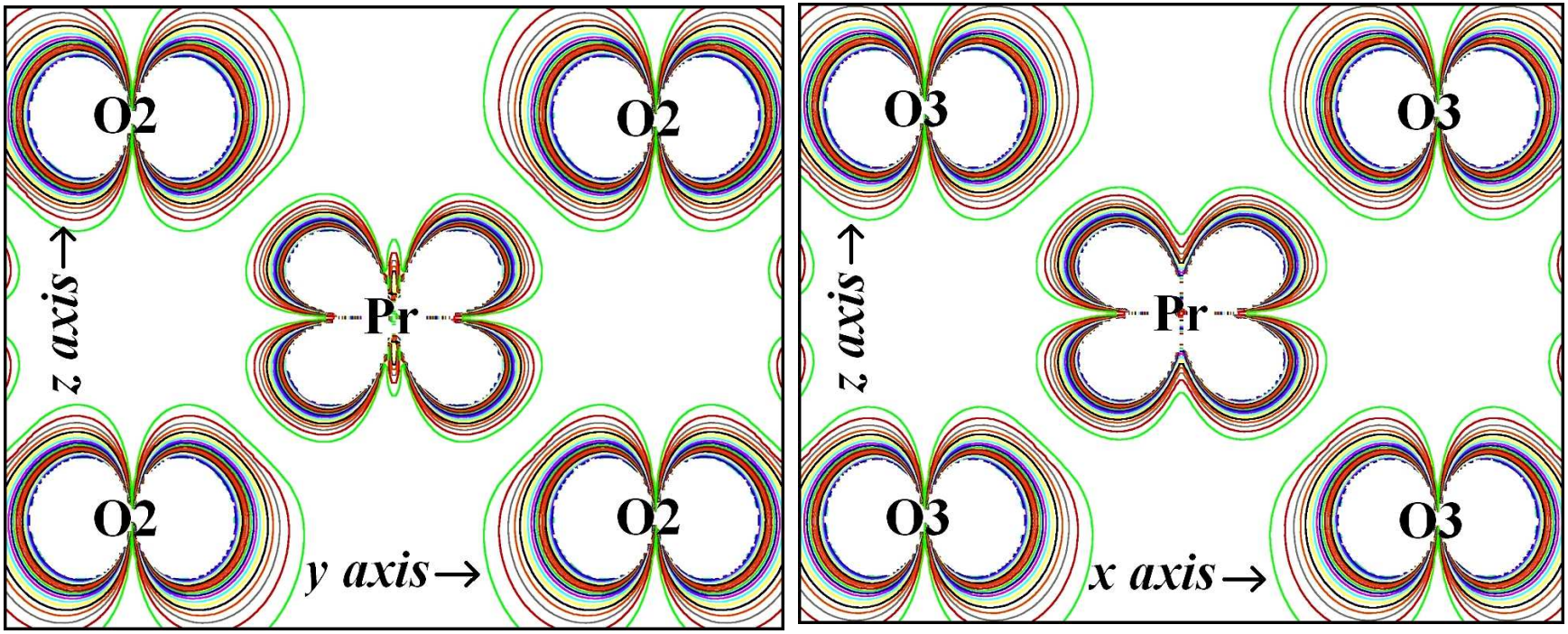

2
1
0
-1
Energy(eV)
E_F
Γ
X
S
Y
Γ
1
2
3
4
5

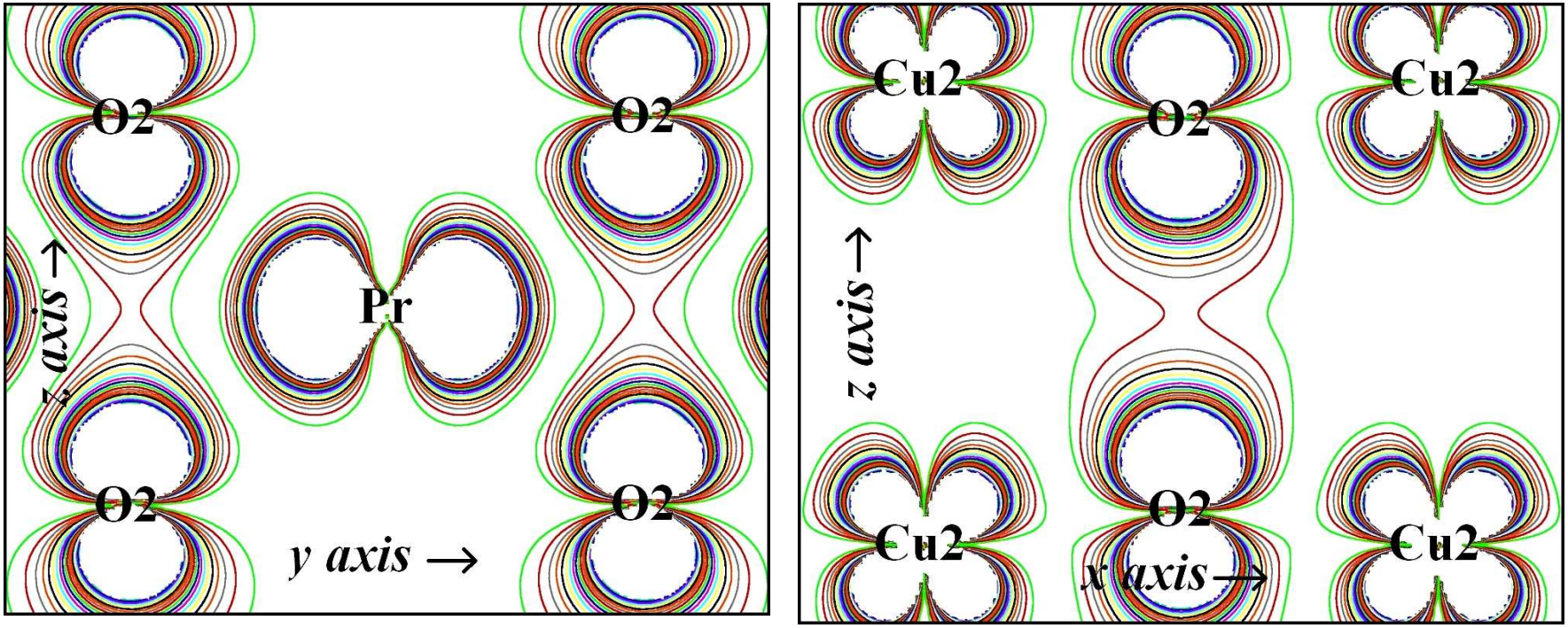

Energy(eV)
2
1
0
-1
E_F
Γ
X
S
Y
Γ
1
2
3
4
5

EFG

	O1	O2	O3	O4
First calculation	17.8	12.7	12.9	12.1
Second calculation	17.7	13.1	13.3	12.2
Experiment: nonsuperconducting Pr123 samples [29]	---	6.9	10.2	11.1

1





V. Ghanbarian , M.R. Mohammadizadeh, submitted to PRB (2008).

Conclusions:

- Y123 ~ Pr123
- ➔ Pr123 is not perfect

Thanks