



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



#### $PrBa_2Cu_3O_7$ جوابهای خودساز گار ساختار الکترونی

محمد رضا محمدی زاده <sup>۱و۲</sup> و حید قنبریان ۱

۱ آزمایشگاه پژوهشی ابررسانایی، دانشکده فیزیک دانشگاه تهران ۲ پژوهشکاده علوم نانو، IPM





- RBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-δ</sub> (R-123)
- Gd : 95.8 K
- Y- : 94.2 K
- Sm- : 93.2 K
- Nd- : 92.2 K
- Dy- : 91.8 K

	GROUP		PE	RI	OD	IC	TA	BL	ΕC	)F <sup>-</sup>	TH	ΕE	LE	ME	ENT	S		18 VIIA
g	1 1.0079						interes and	5 5453 5455	5 GL 1497	512123	119170170		hup:	//www.ktf-sj	olit.hr/perio	dni/en/		2 4.0026
DIN 1	H			RELATIV	/EATOMIC N	(ASS(1)	Me	etal 🚺	Semimetal	Nonme	stal	-						He
Ы	HYDROGEN	2 ILA	GRO	UP IUBAC	PIUDAC GROUPCAS			tali metal		Chalco	igens element	6	13 IIIA 14 IVA 15 VA 16 VIA 17 VIIA				HELUM	
	3 6.941	4 9.0122	ATOMIC N	UMBER-5	10.811			Alkaline earth metal				5 10.811	6 12.011	7 14.007	8 15.999	9 18.998	10 20.180	
2	Li	Be	\$	YMBOL-	OMOL P			l i anthanide	•	Noose :	gas	100	B	C	N	0	F	Ne
	LITHUM	BERYLLIUM	<i></i>	- march	BURGH			Actinide	STAND	- gas	(100 °C; 101 Fe - solid	kPa)	BORON	CARBON	NITROGEN	OXYGEN	FLUORINE	NEON
	11 22.990	12 24.305		_			-		Ga	- liquid	To - synthet	ic	13 26982 14 28088 15 30.974 16 32.065 17 35.45				17 35.453	18 39.948
3	Na	Mg		ELES	MENT NAME			22	NUR.	100			Al	Si	P	S	CI	Ar
	BODAUM	MAGNESUM	3    <b>  </b> B	4 <b>IVB</b>	5 VB	6 MB	7 VIB	8	9	10	11 🖪	12 118	ALUMINUM	SILICON	PHOSPHORUS	BAPHUR	CHLORINE	ARGON
	19 39.098	20 40.078	21 44.956	22 47.867	23 50.942	24 51.996	25 54.938	26 55.845	27 58.933	28 58.693	29 63.546	30 65.39	31 69.723	32 72.64	33 74.922	34 78.96	35 79.904	36 83.80
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
	POTASSILM	CALCIUM	SCANDIUM	TITANUM	VANADIUM	CHROMIUM	MANGANESE	IRON	COBALT	NCKEL	COPPER	ZNC	GALLIUM	GERMANIUM	ARSENIC	SELENRIM	BROMINE	RYPTON
	37 85.468	38 87.62	39 88.906	40 91.224	41 92.905	42 95.94	43 (98)	44 101.07	45 102.91	46 108.42	47 107.87	48 112.41	49 114.82	50 118.71	51 121.76	52 127.60	53 126.90	54 131.29
5	Rb	Sr	Y	Zr	Nb	Mo	Te	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	Ι	Xe
	RUBICAM	STRONTILM	YTTRUM	ZIRCONUM	NICEIUM	MOLYBOENUM	TECHNETIUM	RUTHENUM	RHODUM	PALLADRIM	SILVER	CADMUM	NDRM	TIN	ANTIMONY	TELLUROM	IODINE	XENON
	55 132.91	56 137.33	57-71	72 178.49	73 180.95	74 183.84	75 186.21	76 190.23	77 192.22	78 195.08	79 198.97	80 200.59	81 204.38	82 207.2	83 208.98	84 (209)	85 (210)	86 (222)
6	Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn
	CAESIUM	BAREM	Lanthanide	HAFNIUM	TANTALUM	TUNGSTEN	RHENIUM	OSMIUM	RICIUM	PLATINUM	GOLD	MERCURY	THALLIUM	LEAD	BISMUTH	POLONUM	ASTATINE	RADON
	87 (223)	88 (226)	89-103	104 (261)	105 (262)	106 (286)	107 (264)	108 (277)	109 (268)	110 (281)	111 (272)	112 (285)	1	114 (289)				
7	Fr	Ra	Ac-Lr	Rf	Db	Sg	IBh	IHIS	Mit	Uun	Unn	Uub		Dug				
	FRANCIUM	RADIUM	Actinide	RUTHERFORDUM	DUBNUM	SEABORGIUM	BOHRIUM	HASSEM	MEITNERIUM	UNUNNEUM	UNDINUM	UNUNBUM		UNINGUADUM				
			3	LANTHAN	IDE											Copyright © 19	98-2002 EniG. (	eni@kf-splt.hr
(1) Pure	Appl. Cham., 7	3, No. 4, 667-64	63 (2001)	57 138.91	58 140.12	59 140.91	60 144.24	61 (145)	62 150.36	63 151.96	64 157.25	65 158.93	66 162.50	67 164.93	68 167.26	69 168.93	70 173.04	71 174.97
Relat	tive atomic m ficantifigures Fo	ass is shown or dements have	with five enostable	La	Ce	Pr	Nd	1Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
india	des, the valu ates the mass n	e enclosed in unber of the lor	brackets rgest-lived	LANTHANUM	CERUM	PRAECOVINUM	NEODYMIUM	PROMETHIUM	SAMARIUM	EUROPIUM	GADOLINUM	TERBUM	DYSPROSUM	HOLMIUM	EFBIUM	THULIUM	YTTERBUM	LUTETUM
How	ever three such	elements (Th, F	Pa, and U)	ACTINIDE														
contr tabul	position, and for lated	hose an atomi	e weight is	89 (227)	90 232.04	91 231.04	92 238.03	93 (237)	94 (244)	95 (243)	96 (247)	97 (247)	98 (251)	99 (252)	100 (257)	101 (258)	102 (259)	103 (262)
				Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Ci	Es	Fm	Md	No	Lr
Edito	or: Aditya Verdhi	an (adi wan@nett	Enx.com)	ACTINUM	THOREM	PROTACTINUM	URANUM	NEPTUNIUM	PLUTONUM	AMERICIUM	CURIUM	BERKELIUM	CALIFORNEM	ENSTEINUM	FERMILM	MENDELEVIUM	NOBELIUM	LAWRENCIUM



#### Justifying the insulator behavior of PrBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-8</sub>

Hole filling: Pair breaking: Hybridyzation (FR): Charge transfer: Hybridyzation: LM: Mis-substitution: Semiconductor model: Percolation: Coexistence:

Horn et al., Phys. Rev. B 36 (1987) 3895.
Peng et al., Phys. Rev. B 40 (1989) 4517.
Fehrenbacher & Rice, Phys. Rev. Lett. 70 (1993) 3471.
Khomskii, J. Supercond. 6 (1993) 69.
Wang et al., Phys. Rev. B 50 (1994) 10350.
Liechtenstein & Mazin, Phys. Rev. Lett. 74 (1995) 1000.
Blackstead & Dow, Phys. Rev. B 57 (1995) 11830.
Kakinuma et al., Phys. Rev. B 56 (1997) 3494.
Horii et al., Phys. Rev. B 59 (1999) 3845.

# Superconducting $PrBa_2Cu_3O_{7-\delta}$

Zou et al., Phys. Rev. Lett. 50 (1998) 1074.
 Blackstead & Dow, , Phys. Rev. B 57 (1995) 11830.
 Luszczek et al., Physica C 322 (1999) 57.
 Usagawa et al., JJAP 36 (1997) L1583.
 Shukla et al., Phys. Rev. B 59 (1999) 12127.
 Araujo-Moreira et al., Physica B 284-288 (2000) 1033.

single crystal powders, thin films single crystal thin film single crystal polycrystal





PrCuO<sub>2</sub>



• Small ξ

#### BaCuO<sub>3</sub>

# **Mis-substitution**



**≻** 8.

BaCuO<sub>3</sub>

 $RCuO_2$ 





- 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**

 $(L/APW+lo) \rightarrow WIEN2k DFT$ Exchange-correlation energy → LSDA & LSDA+U **Rotational invariant LSDA+U** → around mean field (AMF) version  $U \& J \rightarrow EFG$ **Ferromagnetic ordering**  $8 \times 8 \times 2$  mesh (200 special k-points)  $\rightarrow$  (16 k-points 1BZ) Plane wave cutoff of  $K_{\text{max}} = 7.5/R_{\text{MT}}$ Charge density  $\rightarrow G_{max} = 14$ R<sub>MT</sub> of Pr, Y, Ba, Cu, and O atoms / 2.8, 2.74, 2.9, 1.8, 0.65 Bohr Total energy → 0.1 meV/Cell



# 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.

$$W = \frac{1}{2} \sum_{i \neq j}^{N} V_{ee}(i, j)$$
$$V_{ee}(i, j) = \frac{1}{4\pi\varepsilon_0} \frac{1}{|\vec{r}_i - \vec{r}_j|}$$
$$\Psi(\vec{r}_1, s_1, \cdots, \vec{r}_N, s_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(\vec{r}_1, s_1) & \cdots & \psi_1(\vec{r}_N, s_N) \\ \vdots & \vdots \\ \psi_N(\vec{r}_1, s_1) & \cdots & \psi_N(\vec{r}_N, s_N) \end{vmatrix}$$

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

Direct Exchange

#### LSDA+U



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

$$N = N_{\uparrow} + N_{\downarrow}$$
 $U = \frac{1}{(2l+1)^2} \sum_{mm'} U_{mm'}$ 
 $J = U - \frac{1}{2l(2l+1)} \sum_{mm'} (U_{mm'} - J_{mm'})$ 
 $U_{mm'} = \langle mm' | V_{ee} | mm' \rangle$ 
 $J_{mm'} = \langle mm | V_{ee} | m'm' \rangle$ 

$${f J}$$
 و  ${f U}$  روشهای مشخص کردن مقادیر  ${f U}$  و

- سعی و خطا وجود کمیت تجربی!
   سازگاری همه کمیتها ی تجربی!
  - تجربی (XPS)
  - ابتدا به ساکن
     تطابق با آزمایش

## مشكلات LSDA+U

- وابسته بودن روش به مقدار U و U
- ابر سلول 🛹 حجم زیاد محاسبات
- مدل: وابسته به نسخه (...-SIC-AMF)
- گاهی پایه اثر گذار است:
   LMTO
   U های متفاوت
   ماتریس عدد اشغال متفاوت







#### EFG

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

case	J <sub>Pr</sub>	U <sub>Pr</sub>	J <sub>Cu1</sub>	U <sub>Cu1</sub>	J <sub>Cu2</sub>	U <sub>Cu2</sub>	Cu1	Cu2	01	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  $\eta$  at oxygen and copper sites of PrBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> for various sets of U and J values in Ry.

case	J <sub>Pr</sub>	U <sub>Pr</sub>	J <sub>Cu1</sub>	U <sub>Cu1</sub>	J <sub>Cu1</sub>	U <sub>Cu2</sub>	Cu1	Cu2	01	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	01	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<sup>-2</sup> and asymmetry parameter  $\eta$  at oxygen sites of nonsuperconducting PrBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$ </sub>, YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$ </sub>, and YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.6</sub>.

		01	02	03	O4
PrBa <sub>2</sub> Cu <sub>3</sub> O <sub>7-5</sub>	EFG		6.9	10.2	11.1
[46]	η		0.09	0.40	0.24
YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7-5</sub>	EFG	17.3	10.5	10.2	11.6
[24]	η	0.41	0.21	0.24	0.32
YBa <sub>2</sub> Cu <sub>3</sub> O <sub>6.6</sub>	EFG		9.4	9.4	11.0
[51]	H		0.23	0.23	0.29



The calculated EFG (Vzz) in units of  $10^{21}$  Vm<sup>-2</sup> and asymmetry parameter  $\eta$  at O2 and O3 sites of Pr(BaPr)Cu<sub>3</sub>O<sub>7</sub> in LSDA

	O2 <sup>-</sup>	O3 <sup>-</sup>	O2‴	03″
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 <sup>-2</sup> at oxygen and copper sites of PrBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub>										
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 ( $\eta$ ) at oxygen and copper sites of PrBa2Cu3O7									
case	Cu1	Cu2	02	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			









#### EFG

	01	O2	03	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



2



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

#### **Conclusions:**

- Y123 ~ Pr123
- → Pr123 is not perfect



