PHYSICAL REVIEW B 81, 229904(E) (2010)

Erratum: Tuning the in-plane electron behavior in high- T_c cuprate superconductors via apical atoms: A first-principles Wannier-states analysis [Phys. Rev. B 79, 214512 (2009)]

Wei-Guo Yin and Wei Ku (Received 24 May 2010; published 9 June 2010)

DOI: 10.1103/PhysRevB.81.229904 PACS number(s): 74.72.-h, 71.10.-w, 74.25.Jb, 74.40.-n, 99.10.Cd

The numbers appearing in Table I were printed without the negative sign where needed. We reproduce the correct table below. Nothing else in the paper has been affected.

TABLE I. Selected parameters in Eq. (1) obtained from the Wannier-states analysis of the LDA+U ground-state electron structures of Ca₂CuO₂Cl₂. D_x stands for $d_{x^2-y^2}$ and D_z for $d_{3z^2-r^2}$. nn denotes nearest neighbor. The unit is eV.

	on-site		1st nn	2nd nn	3rd nn
$\mathcal{I}_{\mathrm{eff}}$	9.625	$T_{ij}^{PsDx} \ T_{ij}^{PsPs} \ T_{ij}^{DxDx}$	-0.388	0.034	-0.092
$J_{ m eff}'$	6.754	$T_{ii}^{P_SP_S}$	-0.288	0.185	-0.076
eff	0.706	T_{ij}^{DxDx}	0.032	-0.003	0.002
1	-0.964	•			
P_S	2.003	T_{ii}^{PsPz}	0.129		0.029
Pa	4.111	T_{ij}^{PsDz}	-0.130		-0.030
$\mathbf{e}_{\mathbf{z}}$	2.812	$T_{ij}^{P_SPa}$	0.065		0.003
PsDx ii	-2.351	T_{ij}^{DxPz}	0.026		0.006
ĎzPa i i	-0.845	T_{ij}^{DxDz}	0.034		0.003
Pz PsDx ij DzPa ij PzPa ij PzDz ij	0.778	T_{ij}^{PsPz} T_{ij}^{PsDz} T_{ij}^{PsPa} T_{ij}^{PsPa} T_{ij}^{DxPz} T_{ij}^{DxDz} T_{ij}^{DxPa}	-0.354		-0.084
PzDz i i	0.951	-,			