COMMENTS

Comments are short papers which criticize or correct papers of other authors previously published in **Physical Review B.** *Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

Comment on ''Superconductivity and Madelung potential of $YBa_2Cu_3O_{6+x}$ ordered superstructures''

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We note discrepancies in numerical results in our calculations of the Coulomb potentials in $YBa_2Cu_3O_{6+x}$ ($x = 0, 0.5, 1$) with those given by Wang *et al.* in ''Superconductivity and Madelung potential of $YBa_2Cu_3O_{6+x}$ ordered superstructures'' [Phys. Rev. B **45**, 10 834 (1992)]. [S0163-1829(96)07830-7]

In the paper by Wang *et al.*[1] the numeric calculations of Madelung potentials in $YBa_2Cu_3O_{6+x}$ crystals are presented and a number of correlations between Madelung potentials of oxygen ions and critical temperature T_c of superconduction transition are formulated. These results are of interest, especially the nontrivial x dependence of Madelung potentials on oxygen — see Fig. 3 and Fig. 5 in Ref. 1, where x is the oxygen concentration. This x dependence is nonmonotonic and nonmonotonic in its first derivative. The nonmonotonic form of the x dependence can be connected with the differences in the geometry of tetragonal and orthorhombic phases of Y-Ba-Cu-O systems. But the nonmonotonic x dependence of the first derivative cannot be explained in this manner due to results given in Fig. 3 of Ref. 1 for orthorhombic states.

Keeping in mind the analytic form of Coulomb potential $1/r$, we can suppose the monotonic dependence of the derivative. Noting the changing x in calculations,[1] we change the distances between oxygen ions in CuO_x planes.

We also cannot answer another question: why Coulomb potentials on apex oxygens decrease as the distance between oxygen ions in CuO_x planes increases (Table II in Ref. 1); that is, as x decreases. This question is not clear, because the potentials on oxygen ions in CuO_2 planes increase with a decrease of x as we can suppose, keeping in mind the analytic form of the Coulomb field.

In order to answer these questions we try to reproduce some calculations performed by the authors of Ref. 1. But we would like to note some inconsistence of the numeric results of Ref. 1 with those obtained by our group. We have calculated the Madelung energies and potentials for a large number of organic and nonorganic materials: TTF-TCNQ, NMP-TCNQ, Rb-TCNQ, BEDT-TTF-J,[2–5] La-Sr-Cu-O, Y-Ba-Cu-O, Tl-Ca-Ba-Cu-O,[6,7] and others. As in Ref. 1 our numeric algorithm is also based on the Ewald method for summing of the long-range Coulomb fields in infinite systems. In this Comment, we present the results of calculations (Table I) of Coulomb potentials and Madelung energies for three structures of $YBa_2Cu_3O_{6+x}$ with $x = 0$, 0.5, and 1 that are selected from the eleven structures considered in Ref. 1. Similarly to Ref. 1, the structural parameters of a tetragonal phase of $YBa_2Cu_3O_6$ and an orthorhombical one of $YBa_2Cu_3O_7$ are taken from Ref. 8 and the parameters of $YBa_2Cu_3O_{6.5}$ from Refs. 9 and 10. We can see that Madelung potentials differ from those given in Ref. 1, comparing our data in Table I with Table II from Ref. 1 .

We conclude that the results of Ref. 1 should be revised. We cannot perform the calculations of the Madelung potentials for all superstructures due to the absence in Ref. 1 of complete data on the geometric charge arrangements in crystals and the mistakes in the chemical formula of compounds given in Ref. 1; these formulas do not satisfy the condition of unit-cell electrical charge neutrality.

Also we have found another mistake in Table II of Ref. 1, where the coefficient between atomic units and electron volts is wrong.

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TABLE I. The calculated values of plane, O(2), and apical, O(4), site potentials (in a.u.) and Madelung energy E_M (in a.u./molecule) of $YBa_2Cu_3O_{6+x}$.

	$x=0$		$x=0.5$		$x=1$	
Atom	Charge	Site potential	Charge	Site potential	Charge	Site potential
O(2) [a]	−2	−1.412	−2	−1.502	−1.75	−1.570
O(2)	−2	−1.478	−2	−1.385	−1.75	−1.588
O(4) [a]	−2	−1.550	−2	−1.388	−1.75	−1.224
O(4)	−2	−1.475	−2	−1.181	−2	−1.175
O(4) [b]			−2	−1.588		
E_M		−9.6274		−10.2828		−10.2850

[a]Values by Wang *et al.* in a.u., q^*V, q is site ionic valence.
[b]The atom with the coordinate $x/a = 1/2$.

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