PESUDOPOTENIAL DENSITY FUNCTIONAL THEORY STUDY OF AU/YBCO INTERFACE

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Résumé
L'interface Au/YBCO est représentée par un modèle simple montrant le contact entre deux surface d'une interface épitaxiale avec la relation d'orientation Au(111)/YBCO(001) où la direction $[011]_{Au}$ est parallèle à $[100]_{YBCO}$; la surface de terminaison du YBCO étant le plan CuO. Un modèle plus simple de l'interface celui Au(001)/YBCO(001) est est utilisé pour calculer les énergies d'interaction entre la couche métallique est le substrat oxyde en fonction de la distance de séparation entre les deux surfaces pour différentes configurations en utilisant la théorie de la fonctionnelle de la densité. La configuration ayant l'énergie d'interaction la plus élevée est celle qui correspond à la situation dans laquelle les atomes d'or sont situés sur les sites oxygène de la surface du supraconducteur.

Abstract
The Au/YBCO interface is represented by a simple model showing the contact of two surfaces of an epitaxial interface with the orientation relationship Au(111)/YBCO(001) where $[011]_{Au}$ is parallel to $[100]_{YBCO}$ for which termination surface of the substrate corresponds to the CuO layer of YBCO. A simplest model with different configuration Au(001)/YBCO(001) is used to calculate the interaction energies using pseudopotential DFT approach as a function of the separation distance between the metallic film and the surface of the superconductive substrate in different configurations. The configuration with the highest interaction energy at the interface Au/YBCO(001) was found to correspond to the deposition of Au film in such way that the Au atoms of the interfacial monolayer are top oxygen atoms of the substrate surface.

I. INTRODUCTION

Since superconductive materials have been discovered in the end of the 1980s application and theoretical studies have been carried out to develop techniques to fabricate superconductive materials and devices. Among superconductive materials the YBCO ($YBa_2Cu_3O_{7-x}$) was the first high critical temperature superconductor HTC with a working temperature of about 77 K. Applications of superconductive materials have been since developed and covered many fields such as NMR devices (working at strong magnetic fields in the range of 3-5 tesla assured by the high currents reaching 10^4 - 10^6 A/cm2 [1-3]), microwave devices [4, 5] Josephson devices [6-15], YBCOsilicon hybrid/integrated electronics and microelectronics device applications [13], HTS based transmission cables [15, 16], motors, generators, SMES, transformers, high-field magnets, high critical temperature magnets [17], electric power application, [18-21], superconducting magnetic energy storage system [22] and fault current limiter [23]. The YBCO superconductive material belongs to the crystallographic family of ceramics known to be very rigid but fragile and chemically unstable when its surface is exposed to atmospheric air [24]. In addition this superconductive ceramics need to be wired to the electric circuit which is mainly realised by metallic contacts. These contacts must have very good quality to ensure carrying high electric currents. Mechanical supporting the superconductive material is ensured by oxide [4, 25, 26] or by metallic substrates [1, 6, 7, 28 - 31]. Among these laters, the gold and silver were the first to be used in such contacts and substrates [6, 27]. The structure of the interface between superconductor and metal controls the electric quality of the contacts [32, 33]. In order to get such metallic contacts with YBCO superconductor metal, has to be deposed on perfect superconductor surface to avoid structural defects. This can be achieved by metal evaporation or sputtering which can yield abrupt interfaces on large surfaces can be realised. A stepped interfaces can be seen also with a step difference of a multiple of constant height which corresponds to the parameter c of the unit cell of YBCO [34] suggesting that a preferential termination of the YBCO (probably CuO one) is in contact with the metal at the interface. Several metal/oxide interfaces have been studied theoretically in the aim to determine their atomic and electronic structure. The examples the Ag/MgO [35], Pd/MgO [36], Ag/Al_2O_3 [37] can be cited here. These studies were carried out using DFT calculations which become more and more involved in the field of theoretical condensed matter studies nowadays. However, such studies are not available for the Au/YBCO interface. To get more comprehension of the atomic structure of this interface we attempt to study the structure of the Au(100)/YBCO(001) interface by the use of DFT calculations in order to determine the surface potential energy (SPE) which can be used to describe the interatomic interactions between the two sides of the interface. The SPE can be used then to simulate the interface structure at a mesoscopic scale. Such work has been done for other interfaces [37, 38]. <Q The paper will be organized like follows: we represent a model of the Aug/YBCO interface which we use then to calculate interaction energies between the metal Ag and

the superconductor and a description of the calculation details. The results will be presented in a separate section followed by discussions and a conclusion.

II. THE MODEL OF Au/YBCO INTERFACE

The metallic film of gold is generally deposited on termination surface of the superconductor. This is similar to the Ag/YBCO interface for which a similar study is reported elsewhere [39]. We have presented a in this study a model based on the epitaxial relationship revealed X ray diffraction at the interface. The model we present here is not very different. The X ray showed that the epitaxial relationship at the interface is of the form Ag(111)/YBCO(001) where $[110]Ag//[100]_{YBCO}$.

Gold and silver are noble metals, and their crystallographic structure is FCC. Furthermore, their chemical structure unit cell parameters are very close to each other: both belong to the column of the periodic table and the unit cell parameter is 4.08 A° and 4.09 for gold and silver respectively. Taking these considerations into account, a simple geometric model of the Au/YBCO is illustrated on figure 2. This model is similar to the Ag/YBCO one and is based on the assumption that the metallic film is deposited on the 'natural termination' of the superconductive substrate, and takes into account the miss-much between the two materials. In fact, the Au has the CFC unit cell with the cell parameter of 4.08A° which very close the silver unit cell parameter, and the YBCO crystallographic structure is perovkstie type with parameters a, b and c equal to 3.81 (3.82) A°, 3.88 (3.89) A°, and 3.67 (3.68) A° respectively [40-42]. When the two surfaces of both material are brought close to each other to form the interface we can envisage that an atom of Au taken as a reference in top oxygen atom and going along the direction of the *a* axis of the YBCO surface, the next Au atom to oxygen will coincide with the third atom. In the b direction, the coincidence will be with the fifth Au atom as we can see in figure 3. The nearest neighbour distance for the Au (111) surface is and; the two distance of first coincidence in the a and b directions can be determined by these two equations:

$$\begin{cases} n_a.a_{YBCO} = (n_a + 1).a_{Au(111)} \\ n_b.b_{YBCO} = (n_b + 1).b_{Au(111)} \end{cases} \qquad (1)$$

Where n_a and n_b are the numbers of unit cell distances in the *a* and *b* directions respectively; they are deduced from the last equation and are equal to 3 and 5 respectively. Our model shows that the best coincidence takes place as follows: In the [100] direction YBCO, if an Au atom of the metallic interfacial layer is top an oxygen atom of the CuO termination surface of oxygen, the next Au atom is distant by 4x2.8911.56 A°. Because of the difference between the metallic and the oxide lattice parameters, the distance between oxygen coincident atoms of the YBCO surface is 3 x 3.81=11.43 A°. This is little bit different in [010] direction: The Au-Au distance is 4x5.0120.04 A° in front of 5x3.88=19.4 A° for O-O distance. To have an epitaxial deposition of Au(111) on YBCO with CuO termination surface, a dilation of the Au (111) surface parameters of 1.12 % and 3.12 % receptively is necessary. The aim of our study is to obtain interaction energies between the metallic film and superconductor substrate. We have used a supercell containing only one unit cell of YBCO and five monolayers of the metal film which gives more realistic situation since the metallic film is thicker and hence avoiding surface effects on interaction energies. The number of atoms in the supercell reduces to only 26 atoms. Note that the (111) and the (100) face for the metallic film are quite similar for this situation, for this reason the model proposed here belongs to the interface Au(100)/YBCO(001) rather than Au(111)/YBCO(001). The mismatch between the metal and the substrate changes to 7 % for the direction a and to 5 % for the b direction of the YBCO respectively. In DFT calculations, the physical system are modelled by a supercell that represents the physical system conserving as long

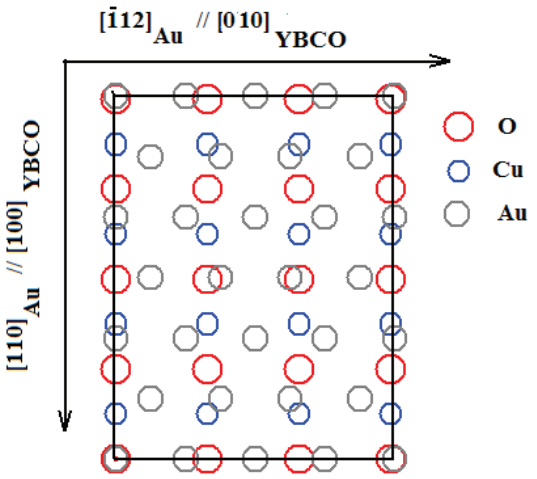

FIG. 3: The model of Au/YBCO interface: the two surfaces Au(111) and YBCO (100) are in contact where $[110]_{Au}$ is parallel to $[100]_{YBCO}$.

as possible its geometrical configuration and chemical composition. If we use the above dimensions of the superconductor as a substrate to depose the metallic film, and taking into account that one unit cell of YBCO counts 10 atoms, the supercell counts 3 x 5 x 10 atoms for the substrate. If we use only three monolayers to represent the Au (111) film we need to use at least three monolayers of Au atoms to simulate a thick metallic film, the three monolayers count 3 x 16 = 48 Au atoms. The total number of atoms in the supercell of our model counts now 198 atoms. This a huge unit cell for the DFT calculations since the computer memory and calculations require powerful machines unfortunately unavailable for us. These values of the mismatch in the last model are quite large compared to model systems of metal/oxide DFT calculations such as Ag/MgO(100) interface in which the mismatch is less than 3 % [38]. However it is reported in many studies of similar

interfaces like Pd/MgO and Ni/MgO where the mismatch is about 7.6 and 16 % respectively [43]. Moreover, the largest mismatch reported in DFT studies is 18 % for the NiO/Ni interface [44]. More first principle studies of complicated interfaces are reported like the Cu/Al_2 O_3(0001) interface in which the mismatch is 7.3 % [45].

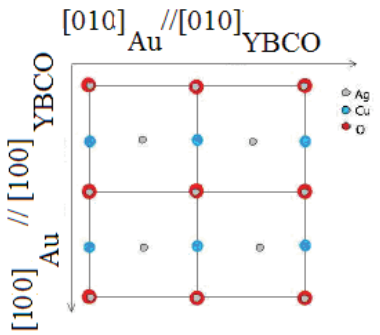

FIG. 4: Model of the Au(001)/YBCO(001): Au(100) and YBCO(001) surfaces are in contact and $[100]_{Au}$ and $[100]_{YBCO}$ are parallel.

III. COMPUTATIONAL DETAILS

In this section we are concerned by the determination of the crystallographic parameters of two materials forming the interface, i. e. Au and YBCO and then the calculation of the separation energy as a function of the distance between the gold film and the substrate surface. We have used two different density functional theory (DFT) methods all electron (WIEN2K code [46]) and PWSCF (Plane-Wave Self-Consistent Field) is a set of programs for electronic structure calculations within Density-Functional Theory and Density-Functional Perturbation Theory, using a Plane-Wave basis set and pseudopotentials [47]) to perform the study of the interface. The all electron and pseudopotential DFT methods were used to stduy the YBCO structure. All electron calculations used both LDA (Local Density Approximation) and GGA (Gnerlized Gradient Approximation) with Perderw-Zhang exchange coorelation. Pseudopotential method was used as follows: for claculations of gold, Perdew-Burke-Ernzerhof (PBE) exch-correlation nonlinear core-correction semicore state d in valence Vanderbilt ultrasoft pseudopotential is used. For Oxygern, Perdew-Burke-Ernzerhof (PBE) exch-correlation Rabe Rappe Kaxiras Joannopoulos ultrasoft pseudopotential is used. For Barium, Perdew-Burke-Ernzerhof (PBE) exch-correlation nonlinear core-correction semicore state s in valence semicore state p in valence Vanderbilt ultrasoft is used. For Yitirium, Perdew-Burke-Ernzerhof (PBE) exch-corr nonlinear core-correc semicore state s in valence semicore state p in valence Vanderbilt ultrasoft PP is used. For Coper, Perdew-Burke-Ernzerhof (PBE) exch-corr semicore state d in valence Rabe Rappe Kaxiras Joannopoulos ultrasoft PP is used. The Vienna university group was one of the pioneers of such studies [48, 49]. Their study was centred on the phonon frequencies in the material. This study implies the structure optimization of the compound [50, 51]. Before the extension of the use of first principle techniques in structure calculations of condensed matter, the semi empirical methods were commonly used. Among these studies, Baetzold and all [52-55] used models based on different basic interatomic interactions like ionic, image-interaction and Vander-Walls interactions and succeeded to reproduce some of important physical properties of the YBCO superconductor like unit cell parameters and oxygen immigration into the material [55]. Recently, Pseudopotential density functional theory study of this material was reported [59]. Some of its electronic structure properties like charge density distribution and density of states were determined in this study. Theoretical studies of interfaces including the YBCO superconductor are fewer and are mostly concerned by the quantum phenomenons [56, 57].

IV. THE STRUCTURE PARAMETERS AND CHOICE BETWEEN LDA AND GGA

The most known two varieties of both pseudopotential and all electron density functional theory are LDA and GGA to deal with the exchange correlation part in the Kohn-Sham equations for Local Density Approximation and Generalized Gradient Approximation respectively. It is well known that GGA is more adequate to transition metal structure and electronic properties calculations [57]. For the YBCO, the available studies indicate that both LDA and GGA were used and gave reasonable results [50, 51]. Moreover, it is noted that GGA approximations gives more reliable image for the charge distribution and phonon frequencies for the antiferromagnetic insulating fundamental state than using LDA in the all electron method [50]. For these reasons, we have chosen the GGA approximation for both pseudopotential and all electron methods. The pseudopotential has been tested by calculating the unit cell parameter for gold and the results was similar to the conclusions given above. The cut-off and k points mesh were optimized using experimental unit cell parameters a, b, and c of the YBCO unit cell for the two varieties of the DFT and found to be 25 eV for the cut-of energy and 8x8x8 for the k points mesh. The pseudopotential data files for the Au, Y, Ba, Cu and O atoms used here are given in [59].

V. $YBa_2Cu_3O_{7-x}$ STRUCTURE OPTIMIZATION

The YBCO denotes the complex high critical temperature superconductor compound with the chemical structure $YBa_2Cu_3O_{7-x}$. The parameter x varies from 0 to 1 meaning that the unit cell counts from 6 to 7 oxygen atoms [60]. This means that in in bulk material some oxygen atoms are missed in the O(1) positions (figure 5).The unit cell structure is composed by 7 planes which are symmetric with respect to the Y plane (plane 4 in figure 5). The positions of atoms in planes 2 and 3 are not aligned which makes the structure calculations quite difficult since it requires atoms positions optimization. This task can be achieved by DFT molecular dynamics applied on unit cell atoms. Note here that if the atoms positions are changed, the

unit cell parameters must be re-optimized again. As we have done for gold, we began the structure optimization of YBCO structure using its experimental data (a=3.82 A°, b=3.89 (3.88) A° and c=11.68 A° and atoms positions in table I). First, unit cell parameters are optimized as follows: Taking two of the three parameters b and c for example equal to their experimental values, the first estimate of the third parameter is that value corresponding to minimal energy versus unit cell volume. This procedure is repeated for the two b and c respectively taking in each time the optimized values for the other two parameters. Once the three parameters are calculated, the second step is launched: the positions of all atoms are recalculated by looking for equilibrium position for each atom in the unit cell. These two steps are repeated until getting convergence of all values of unit cell parameters and atomic positions. The calculated quantities are given in tables I and II.

VI. Au/YBCO(001) INTERFACE

The Au/YBCO(001) interface supercell structure is illustrated in figure 4. If we keep YBCO unit cell parameters a and b unchanged; and atoms of gold are top corner atoms of CuO termination surface of YBCO; this leads to a contraction of the unit cell with horizontal parameters $a_{Au} = a_{Y\ BCO}$, $b_{Au} = b_{Y\ BCO}$. The effect of such contraction which is about 7 % on gold is compensated by the dilatation in the direction parallel to c parameter. To perform these calculations, gold horizontal parameters *a* and *b* taken equal to those of YBCO to dilate the perpendicular metal interlayers distance, this is achieved by an optimization of c_{Au} parameter by seeking the minimal energy versus volume. The obtained value is found to be 4.65 A° (figure 6). In order to calculate the interaction energies between metallic film and superconductive substrate, the supercell can be constructed in different ways depending on the relative positions of the gold atoms of the interfacial layer and the YBCO surface termination. Among These configurations, three of high symmetry are illustrated in the figure 7. These configurations will

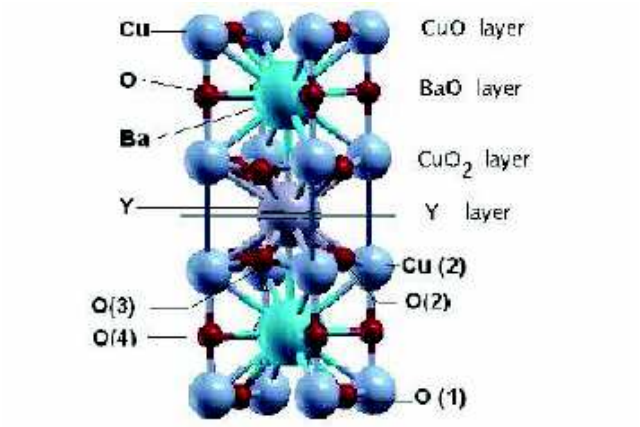

FIG. 5: Structure of unit cell of YBCO superconductor, Atoms of planes 2 and 3 are ont aligned.

TABLE I: Unit cell parameter of YBCO calculated using GGA and LDA in the frame of all electron (WIEN2k code) and pseudopotential(code PWSCF) DFT approaches.

	All electron	Pseudo -potential	Experimental
Unit cell parameters a, b and c (A°)	3.75, 3.80, 11.45(LDA) [50] 3.83, 3.95, 11.71 (GGA, this work)	3.81, 3.93, 11.74 (GGA, this work)	3.82, 3.89 , 11.68 [50] 3.83, 3.88, 11.68 [61]
Bulk modulus B (GPa)	142 [50] 121, 229 (this work, WIEN2K code)	103 (this work, PWSCF code)	27, 107,196 [50] 148 [62]

TABLE II: YBCO atoms positions from all electron (A.E.) and pseudopotential (P.P.) *DFT*, semi-empirical (S.E.) calculations, and experimental data.

	A.E LDA) [49]	A.E. (GGA) (this work)	P.P. (GGA) (this work)	S.E. [52]	. Exp. Data [52]
Volume ($A^{°3}$)	163.1	176.2	171.3	170.6	173.5
c/a	3.015	3.073	3.057	3.0127	3.052
b/a	1.	1.031	1.032	1.0157	1.016
z_{Ba} (c)	0.1817	0.1800	0.1800	0.1876	0.1843
$z_{Cu(2)}$ (c)	0.3507	0.3516	0.3514	0.3556	
$z_{O(2)}$ (c)	0.3765	0.3781	0.3780	0.3800	0.3789
$z_{O(3)}$ (c)	0.3770	0.3779	0.3780	0.3801	0.3773
$z_{O(4)}$ (c)	0.1619	0.1609	0.1609	0.1607	0.1584

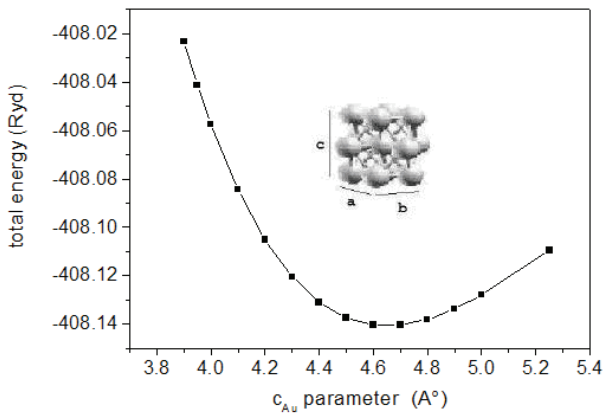

FIG. 6: Calculation of the parameter c of tetragonally deformed gold with a and b parameters taken equal to those of the YBCO unit cell. The curve with filled square belongs to a second optimization with a cut-off of smaller value than reported above.

be used to determine the interaction between gold film and YBCO. Intermediate situations can be calculated using appropriate interpolation functions that take into account the surface symmetries and will be discussed in a separate section. The first configuration of the interface is related to the situation in which Au atoms are top Cu atoms of the CuO surface while the second one is that situation where two of Au atoms are top oxygen ones (situated in the middle of *b* axis) while the other atoms of Au unit cell surface are located on vacant sites along a axe of the YBCO surface. The third configuration concerns an intermediate situation between configuration 1 and 2 and where the gold atoms are situated on the centre of the triangle made by the Cu atom, O atom and the CuO surface centre site (see situations (a), (b), and (c) respectively of the figure 7). In addition to the horizontal relative positions of the atoms at the interface, the determination of the surface potential energy require the calculation of the interaction energy on the separation distance between gold and superconductor surface. This calculations lead to determine the equilibrium distance for each one of the three configurations discussed above. To obtain the interaction energy for a given configuration and separation distance, we calculate three total energies belonging to Au and YBCO slabs and the interface Au/YBCO(001) respectively (figure 8).

VII. RESULTS AND DISCUSSION

The total energy of the supercell we used to model the interface can be given by

$$E_{tot} = E_{YBCO}^{slab} + E_{Au}^{slab} + 2E_{\text{int}} \qquad (2)$$

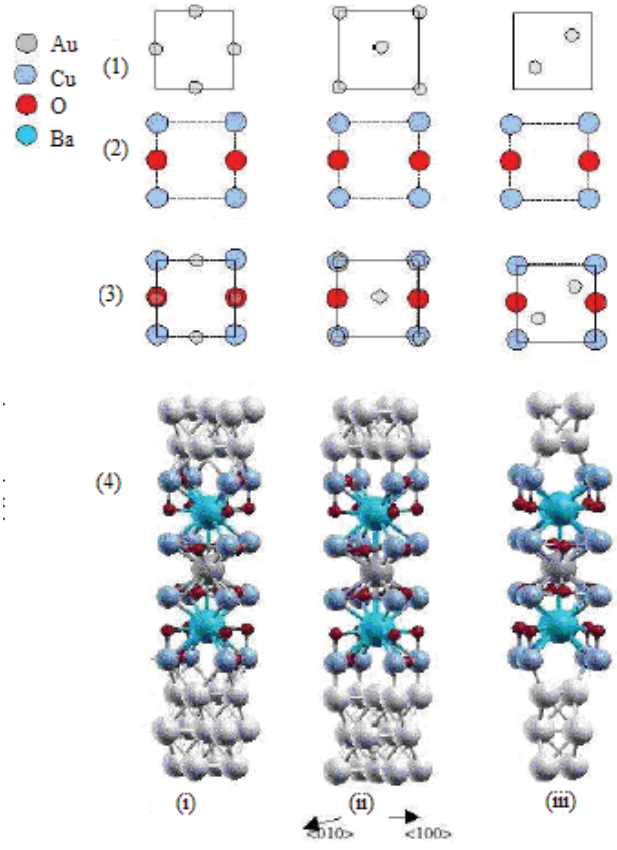

FIG. 7: Structure of Au(001) and YBCO(001) surfaces with CuO termination: (1) and (2). The three configurations of high symmetries: (i) Gold atoms are top oxygen sites, (ii) Au atoms are top copper atoms, and (ii) Au atoms are top intermediate sites, (3) surfaces in contact and (4) 3D supercell of the interface.

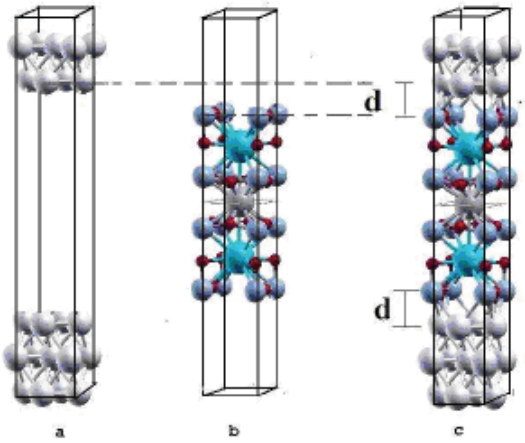

FIG. 8: Systems used to calculate interaction energy at the interface: a) and b) separated systems with surfaces and c) the supercell representing the interface Au/YBCO(001) with a distance of separation vertical to the contact surfaces.

Where E_{tot}, E_{Au} and E_{YBCO} denote total energies of the Au/YBCO(001) and separated Au and YBCO systems respectively. Factor two in this formula is related to the presence of two interfaces in the supercell. The interaction energy for a given separation distance d is then obtained from equation 2:

$$E_{\text{int}} = \frac{1}{2}(E_{tot} - E_{YBCO}^{slab} - E_{Au}^{slab}) \qquad (3)$$

In figure 9, we represent the results of calculated interaction energies of the Au/YBCO(001) interface using *DFT* pseudopotential approach. It includes the dependence of the interaction energy on the separation distance for the three different configurations in relation with the position of the gold interfacial layer atoms with respect to the CuO surface atoms. As we can see on these curves the most stable situation of the interface is that in which the Au atoms are top oxygen atoms with attractive interaction energy of about 1.09 eV/u.s. and a separation distance of 2.20 A°. However; the smallest interaction energy is that related to the situation where gold atoms are positioned top Cu atoms with energy of 0.72 eV/u.s. and a separation distance of
2.59 A° (see table III). This results are quite different from those obtained for the Ag/YBCO(001) interface, where the interaction energy for the third configuration was less pronounced compared to the present one[39].

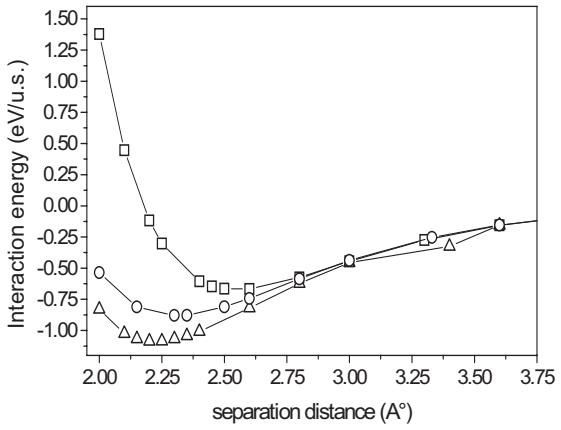

FIG. 9: Interaction energies curves as a function of separation distance (d) at the interface Au/YBCO of the three configurations (figure 7) calculated using pseudopotential DFT approaches. Circles, triangle, and squares denote the calculated interaction energies for the situations of gold atoms top oxygen, copper

TABLE III : Distance of separation and interaction energies at the Au/YBCO(001) in the three configurations

Site	distance of separation (A°)	Interaction energy (eV/u.s.)
O	2.20	1.09
Hollow	2.31	0.92
Cu	2.59	0.72

XI. CONCLUSIONS

The geometrical configuration of the Au/YBCO interface was presented by a simple model made by the contact of two surfaces of an epitaxial interface of the orientation relationship Au(111)/YBCO(001) where $[011]_{Au}$ is parallel to $[100]_{Y\ BCO}$. To calculate the interaction energies at this interface, a simplest model with different configuration Au/YBCO(001) is presented and used to calculate the interaction energies using DFT pseudopotential. The proposed model of the interface is used to get an estimation of the interaction energies and their dependence on the separation distance between the metallic film and the surface of the superconductive substrate with CuO termination. The relative horizontal positions of the interfacial Au monolayer with respect to the substrate surface atoms representing three different situations of high symmetries on the surface: (1) Au atoms are top oxygen atoms,(2) Au atoms are top copper atoms, and (3) Au atoms are top intermediate sites. The calculated interaction energies show that the most stable configuration of the interface Au/YBCO(001) is that corresponding to the situation in which the Au film so that the Au atoms of the metallic interfacial monolayer are top oxygen atoms of the substrate surface with an interaction energy of about 1.09 eV/u.s. and a separation distance of about 2.20 A°.

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