# **Geometrías optimizadas de los clusters de óxidos metálicos de 48 átomos.**

***Geometría para óxido de cobre (CuO).***

Cu O

1.00000000000000

28.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 28.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 28.0000000000000000

Cu O

24 24

Selective dynamics

Direct

0.3893326396908887 0.4602824075564211 0.5886529433920232 T T T

0.3462942525306985 0.4050867501131734 0.5192385294037600 T T T

0.3855532007177284 0.5438775341651011 0.5068519566650436 T T T

0.3809169424533816 0.4675985063816482 0.4410937551183392 T T T

0.4185329267595378 0.5606640858950079 0.4256769293589205 T T T

0.4529649478579580 0.4028801019558297 0.5899558207512275 T T T

0.4380798095013069 0.5532266249353708 0.5976921221068177 T T T

0.4239992372448065 0.3808593949536669 0.4967911338701201 T T T

0.4632165450304544 0.4711030769454118 0.4931228209778830 T T T

0.4599500065648742 0.5974749355725247 0.5040183580406870 T T T

0.4720075800709805 0.4139146012802533 0.4004698889779710 T T T

0.4863081180240617 0.5133342282385771 0.3719790163826638 T T T

0.5179528765320619 0.4837289603559692 0.6236071569669502 T T T

0.5318365381943524 0.5841043504993324 0.5955636391437629 T T T

0.5392376003576060 0.4053172041059317 0.4951315336296372 T T T

0.5418196449959964 0.5305571565279976 0.5000000067740018 F F F

0.5735840347312751 0.6248185449053274 0.5024462420027241 T T T

0.5646784229968810 0.4496558993888694 0.4003290478632368 T T T

0.5469012859619025 0.5974449557070127 0.4100297134260590 T T T

0.5810974352722083 0.4403511199662477 0.5687404305336545 T T T

0.6243510758513817 0.5328800605447108 0.5616777509920285 T T T

0.6160526118217544 0.4592484782957447 0.4885928941452941 T T T

0.6459657576842543 0.5908831636147929 0.4809833731906526 T T T

0.6117745316280347 0.5407956437894106 0.4046470599856151 T T T

0.3355033638860450 0.4287999302136351 0.4640383811821309 T T T

0.3926558730395507 0.5141110785823602 0.6216313832997813 T T T

0.3892918242575968 0.3857247823640252 0.5643028765117130 T T T

0.4002137645580732 0.4788154694016819 0.5216015092467213 T T T

0.4073540090207620 0.5926445189754751 0.5498091437759002 T T T

0.4359201587355832 0.3716720610295451 0.4355000919841223 T T T

0.4283358844272461 0.4998184007210009 0.4069905421401584 T T T

0.4141716283262835 0.6144955667410789 0.4573916505450143 T T T

0.4787794616607051 0.4355687301774580 0.6359461874756963 T T T

0.4930814097387770 0.5498049381334985 0.6358941863613405 T T T

0.4788450248847065 0.4002151598822981 0.5284007357894389 T T T

0.4930824296838152 0.5569253333662900 0.5430841409200181 T T T

0.5073757971164627 0.4497945766017904 0.4502360737174844 T T T

0.5178626803865041 0.5999931338332793 0.4714211004106629 T T T

0.5073299604941722 0.4499029570368056 0.3573719718661915 T T T

0.5214280666280202 0.5642907824669695 0.3607245808599156 T T T

0.5787654287870937 0.3854372890912440 0.5430172594053042 T T T

0.5783786855702207 0.4999228233236843 0.5931028992054558 T T T

0.5644941108152494 0.6287936161116561 0.5645295172631083 T T T

0.5926510275316685 0.4074067609304134 0.4502558362627258 T T T

0.6069308454964212 0.5216503588153136 0.4716478673871042 T T T

0.6140638765083916 0.6140700122053497 0.4287486591807789 T T T

0.6141208920726262 0.4854718771208469 0.3783543659281303 T T T

0.6645540551774374 0.5716461922714698 0.5359761518738302 T T T

***Geometría para óxido de níquel (NiO).***

O Ni

1.00000000000000

28.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 28.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 28.0000000000000000

O Ni

24 24

Selective dynamics

Direct

0.6358667868389674 0.6431145379811767 0.5001715212780269 T T T

0.6430672087793496 0.5645821459040974 0.5645493379917355 T T T

0.6431045835264513 0.5645838609831060 0.4284085322801303 T T T

0.6428744092289378 0.4356955920679795 0.5678653168589634 T T T

0.6430640906358178 0.4354391786657530 0.4354327224069081 T T T

0.6358614000794205 0.3569058847792022 0.5001755144125184 T T T

0.4212242471478618 0.4216775882424173 0.5002029293735504 T T T

0.4283288071547346 0.5001794851999506 0.4287831430651963 T T T

0.4283251910512433 0.4997935563302818 0.5712189685111397 T T T

0.4212314339331371 0.5783407484016720 0.4997901389712496 T T T

0.5003906741184565 0.3568667203533309 0.5001560516468331 T T T

0.5002626016497729 0.4283409939340572 0.4283676366603189 T T T

0.5001995433157660 0.4283049754100716 0.5784141464163852 T T T

0.5001887214919236 0.5069329632147799 0.3568088033278798 T T T

0.4999999919049998 0.4999999919049998 0.4999999919049998 F F F

0.5001808953581843 0.4930742941253854 0.6431744188349384 T T T

0.5001990839249331 0.5717228562138885 0.4216126862664140 T T T

0.5002649831595036 0.5716826226685612 0.5716252144902683 T T T

0.5004009001871239 0.6431637777460608 0.4998457976257313 T T T

0.5715751284175852 0.4217058051107685 0.4998197995564340 T T T

0.5716709294235613 0.4998091564824207 0.4283865493209973 T T T

0.5716683044563098 0.5002182100575965 0.5716029682091914 T T T

0.5716043396695127 0.5783175241176579 0.5001724922646886 T T T

0.6502060886291190 0.4998459879746449 0.5001931728276503 T T T

0.4380775817790479 0.3570525728373966 0.4999915014980161 T T T

0.4356297767563575 0.4290066256176956 0.4321430867039453 T T T

0.4327304978507698 0.4294103263123787 0.5707643416241481 T T T

0.4256703182675778 0.5000908832328435 0.4998645151124350 T T T

0.4327108745705814 0.5708736898638165 0.4292727123097109 T T T

0.4355183706828853 0.5680487640456704 0.5715709846358479 T T T

0.4380382356288237 0.6431441140561773 0.4997957499622956 T T T

0.5003292809983151 0.4253421897534153 0.4999357811608149 T T T

0.5002091967090720 0.4340079052387011 0.6429892063231080 T T T

0.5002215509264616 0.4966991317189908 0.4217229288759441 T T T

0.5005879338058961 0.5031087477497991 0.5780720481170007 T T T

0.5005870220967239 0.5662238648148517 0.3566692375396840 T T T

0.5002596185979158 0.5748929228744046 0.4999260049620418 T T T

0.5713230056193908 0.3536070945457155 0.4999320948734365 T T T

0.5750811998408238 0.4288567302901285 0.4285499705748492 T T T

0.5785393370869443 0.4285243437184434 0.5751159678138009 T T T

0.5749592969452806 0.5000545217984467 0.4999648235387113 T T T

0.5785550534795334 0.5715345390448263 0.4247961713230666 T T T

0.5750297730090921 0.5713482519406696 0.5714020759117844 T T T

0.5712918715107378 0.6465389762769362 0.5000095097438049 T T T

0.6465979495072958 0.4221016386822853 0.5000680992690576 T T T

0.6464146968097353 0.4999195821166040 0.4287311103478473 T T T

0.6463686714241703 0.5001612575749874 0.5710052565612358 T T T

0.6465615617320069 0.5781393530276731 0.4997294749036598 T T T

***Geometría para óxido de zinc (ZnO).***

O Zn

1.00000000000000

28.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 28.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 28.0000000000000000

O Zn

24 24

Selective dynamics

Direct

0.6783122658239714 0.5283371370039874 0.4716632628010794 T T T

0.5574063442434013 0.3288145664627001 0.4716119908461181 T T T

0.4357031898963568 0.3321626617284476 0.4714306341959944 T T T

0.3571487027666327 0.4321527960129694 0.4428608088096096 T T T

0.3788200819168383 0.5712252850743628 0.4002492089139525 T T T

0.3783590221737841 0.5428377615236037 0.5283100574060604 T T T

0.4426243595000980 0.4715951008120136 0.3574223890389613 T T T

0.4431253066466532 0.4645261285111282 0.5501090773798664 T T T

0.4500048684682405 0.5250103855647856 0.4500093816328560 T T T

0.4707319856462018 0.5358368294482430 0.6286716448738870 T T T

0.4998513401397836 0.3645194834222792 0.3645399078688105 T T T

0.5073056650261819 0.3787947791581226 0.5430666661129362 T T T

0.5035694037434323 0.4285850130916446 0.4500008759233008 T T T

0.5002064167014850 0.4427192690051057 0.6426446505415238 T T T

0.4997906732061060 0.5712826023443376 0.3503064845273828 T T T

0.4926460605477402 0.5783663519567497 0.5430674132301615 T T T

0.5073712291801693 0.6426500663332817 0.4502523908787852 T T T

0.5572796862649126 0.4645420824689438 0.3574121044920854 T T T

0.5641024556221369 0.4788003869219313 0.5430671939801637 T T T

0.5573156623237543 0.5359204245579438 0.4502546710704976 T T T

0.5154944721475679 0.5359074945868187 0.6321484846456157 T T T

0.6497138828448640 0.4145076239696320 0.4287885757954182 T T T

0.5997196331746484 0.5859313554249119 0.3788193185800877 T T T

0.5926601011474170 0.5930862284305284 0.5354557703058496 T T T

0.3509481877574781 0.4837474228047215 0.5009862974368999 T T T

0.3929358839388362 0.4576776529860903 0.3957551876874995 T T T

0.3945488003323808 0.3779283622942247 0.4604224170464729 T T T

0.3851220248560859 0.4359040490832753 0.5621133946845109 T T T

0.3893665970636334 0.5645060073727846 0.4642268536458917 T T T

0.4571849770500230 0.4645474603311048 0.4822519230442767 T T T

0.4406047532257989 0.5432740838060316 0.3786383870054260 T T T

0.4358185977164495 0.5340820319429223 0.5642481452318765 T T T

0.4404763748782989 0.6579089598876229 0.4857706878001518 T T T

0.4993338181505834 0.3545469128721231 0.4789290699419978 T T T

0.4956246562971124 0.4290327517241636 0.3719866143444006 T T T

0.5066471000328318 0.4331822866085221 0.5785674620272079 T T T

0.5000017964360026 0.5669982097420032 0.4754500017269976 F F F

0.5256089527396071 0.6141949610039856 0.3923434725234471 T T T

0.4882724345371779 0.6433370143792321 0.5647073096083449 T T T

0.5496011528596932 0.4718447725884120 0.4754553322702044 T T T

0.5566605717080880 0.5331902440468224 0.3711714005520056 T T T

0.5500165752378867 0.5430708740563807 0.5677878514865393 T T T

0.5535260884411745 0.6355962104556879 0.5002091378045135 T T T

0.6037277284470007 0.3715466480022052 0.4710630259792680 T T T

0.6070822614929925 0.4394014410159064 0.3858937952785919 T T T

0.6141525190054089 0.4324224199921869 0.5429083987266246 T T T

0.6213021962772459 0.5573555196708019 0.4822996689769845 T T T

0.6675534969883913 0.4646984237565909 0.4714038915771067 T T T

# **Geometrías optimizadas de los clusters de óxidos metálicos de 18 átomos.**

***Geometría para óxido de cobre (CuO).***

Cu O

1.00000000000000

26.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 26.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.0000000000000000

Cu O

9 9

Selective dynamics

Direct

0.4294195689471252 0.4775808385895175 0.4771209530626805 T T T

0.4689198979105313 0.4617120863678394 0.3848811257288673 T T T

0.5290048696391523 0.4515392701449414 0.4697965738774812 T T T

0.4563467097732499 0.5620738592528625 0.3599019462805728 T T T

0.4168059243647093 0.5776877794033766 0.4483964316573861 T T T

0.5385549843633655 0.5126280955612330 0.3414396659284051 T T T

0.5266057692309971 0.5439923076920010 0.5000000000000000 F F F

0.5112185686333390 0.6112944249947461 0.4274789601145841 T T T

0.5952925813052730 0.5280958456229996 0.4280071874073030 T T T

0.6028709616841752 0.5229617505245585 0.3606827060973501 T T T

0.4680844879305539 0.4241568867018302 0.4443710707384341 T T T

0.3811758436585180 0.5256903018183507 0.4752123509472099 T T T

0.4704095542507716 0.5014308495129143 0.3261967650159789 T T T

0.4866975917256013 0.4885202322583737 0.5216548784225381 T T T

0.4465841812573714 0.6210189571247184 0.3978594830750666 T T T

0.4753176432057700 0.5929960854610812 0.4930043773663613 T T T

0.5809211946594104 0.4957714236474402 0.4909524901331608 T T T

0.5695749831474828 0.5887633557055025 0.4614577422055035 T T T

***Geometría para óxido de níquel (NiO).***

Ni O

1.00000000000000

26.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 26.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.0000000000000000

Ni O

9 9

Selective dynamics

Direct

0.4019344471010403 0.4401405658340738 0.4696844223397116 T T T

0.3617696778414972 0.5143089449398368 0.4173757261226428 T T T

0.3917878558510846 0.5176040184998635 0.5379494626993604 T T T

0.4523221227790166 0.4608161933922152 0.3659930489705611 T T T

0.5000000000000000 0.5000000000000000 0.5000000000000000 F F F

0.4472380663177213 0.5914308568775368 0.3840368050887690 T T T

0.4620071980085591 0.6090469031660969 0.5538128540057488 T T T

0.5364737626393423 0.5316612602366927 0.3898250527526542 T T T

0.5281560857945492 0.6080356689288240 0.4637000206253348 T T T

0.3951692306769042 0.4473023902964035 0.3988343667364174 T T T

0.3518998756736976 0.4915653040867277 0.4846217713907371 T T T

0.4467999530130852 0.4646933563685152 0.5204675771250680 T T T

0.3866194635981896 0.5688396893165583 0.3840228385133320 T T T

0.4141704548654344 0.5699710671696603 0.5743649214506790 T T T

0.5111604791531709 0.6379858389583372 0.5218299300063489 T T T

0.5121275310211043 0.4811469478718481 0.3506386884631361 T T T

0.5441197552116152 0.5339855379750778 0.4630630887727003 T T T

0.5135021977575723 0.6022966178369394 0.3922961360614886 T T T

***Geometría para óxido de zinc (ZnO).***

O Zn

1.00000000000000

26.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 26.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.0000000000000000

O Zn

9 9

Selective dynamics

Direct

0.5034324620919790 0.6035821806181190 0.3557403066873874 T T T

0.4296478913933868 0.7024263201832426 0.4534095568886656 T T T

0.5183884805297652 0.6335938161081955 0.4634369978363608 T T T

0.3979112400616813 0.6120110142220199 0.3940289446661893 T T T

0.5372563262815007 0.5226631854135420 0.4633257947939953 T T T

0.4631301173026827 0.6210958847602583 0.5609763414816200 T T T

0.4183639047486238 0.5010649763967265 0.3947110213020721 T T T

0.3442062158893862 0.6000300007136232 0.4923209963015864 T T T

0.4318958031587670 0.5299469171419418 0.5027317863628937 T T T

0.4664508235023206 0.6524516229911939 0.4050488269084909 T T T

0.5394000977147471 0.5778775876393780 0.4145949836387359 T T T

0.4688812999352052 0.6721025298642473 0.5079830980400288 T T T

0.4436000645006217 0.5606745798306036 0.3594733605468079 T T T

0.3731763081936137 0.6551375113514268 0.4529024618181410 T T T

0.5000000000000000 0.5721519230770014 0.5117980769230002 F F F

0.3817447623177017 0.5508439688874773 0.4435910440716100 T T T

0.4709277053408414 0.4955716895021638 0.4460631584616337 T T T

0.4000230781437892 0.5896514381684383 0.5393125003180614 T T T