

Supporting Information

Zinc doped boron phosphide nanocluster as efficient sensor for SO₂

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Cartesian Coordinates of the Optimized Structures

B₁₂P₁₂

Symbol	X	Y	Z
B	-2.43763300	-1.17136700	0.00096900
B	-0.44854100	-0.83308500	-2.33606700
B	-0.44024500	-2.61619000	0.00371300
B	-0.44798400	-0.82507200	2.33877600
B	2.14043500	-1.78327200	-1.17954200
B	2.14040300	-1.77963300	1.18463000
B	3.06642000	0.80340700	-0.00144000
B	1.30317900	0.82134400	2.38080600
B	1.30275900	0.81396400	-2.38317500
B	1.47432500	2.55724800	-0.00395600
B	-1.24426200	1.93358000	1.14715800
B	-1.24456400	1.92981900	-1.15248400
P	1.39820600	-3.11422200	0.00458900
P	3.48008300	-1.05991100	0.00142500
P	1.42050900	-1.06615600	-2.79529900
P	-1.57383900	-2.10191000	-1.47675400
P	-1.57312700	-2.09561900	1.48214200
P	-0.57833500	1.05583100	-2.71492800
P	-2.70782600	1.57197900	-0.00194000
P	-0.32521900	3.18047100	-0.00482400
P	-0.57777500	1.06472400	2.71249600
P	1.42098900	-1.05755200	2.79848100
P	2.55364400	1.94490500	1.46970700
P	2.55339300	1.94044000	-1.47601500

B₁₂P₁₂-SO₂

Symbol	X	Y	Z
B	-2.30816000	-0.79794400	0.97362100
B	0.24846100	-1.29403800	2.36063600
B	-1.10331200	1.36872300	1.75743700
B	-1.35396800	1.86686400	-1.00106900
B	1.92755500	1.07805300	1.92675300
B	1.19760900	2.59404400	0.24479700
B	2.97976300	0.44037600	-0.77167300
B	0.61847700	1.30329700	-2.33192700
B	2.16614500	-1.75949700	1.07455500
B	1.85257200	-1.34590700	-1.85456900
B	-1.12827600	-1.11423300	-1.85080000
B	-0.38219000	-2.65727400	-0.27494800
P	0.51167700	2.38552500	2.03252700
P	2.96669400	1.86350800	0.50260300
P	2.04052600	-0.67951800	2.67056000
P	-1.39902100	-0.36603200	2.56238200
P	-2.50855000	1.81100500	0.50337500
P	0.62468600	-2.89010200	1.34293800
P	-2.20260900	-2.07206200	-0.52876500
P	0.27541400	-2.40254700	-2.06984500
P	-1.19033700	0.66850900	-2.53381500
P	0.22947400	2.92276500	-1.35931300
P	2.27710200	0.38945900	-2.57372200
P	3.20954000	-1.45659000	-0.49463100
S	0.27557493	0.60974925	4.39312558
O	1.62050158	0.23775841	4.83492500
O	-0.87623921	-0.11965567	4.92574573

B₁₂P₁₂-Zn (M1)

Symbol	X	Y	Z
B	-2.00524000	-2.15227400	-0.00000900
B	-0.29642600	-1.04502000	-2.18236500
B	0.32705900	-2.87037800	-0.00004600
B	-0.29641900	-1.04512100	2.18232400
B	2.51970100	-1.27363200	-1.16840500
B	2.51970300	-1.27367600	1.16835700
B	2.79285500	1.46561300	0.00002500
B	0.99989100	1.03483100	2.26375300
B	0.99989000	1.03491800	-2.26373000
B	0.87872400	2.85140900	0.00005100
B	-1.82084800	1.76426500	1.04143400
B	-1.82084000	1.76431300	-1.04138800
P	2.22329800	-2.77306000	-0.00005100
P	3.64743000	-0.23699700	-0.00000600
P	1.55236600	-0.75074100	-2.73563900
P	-0.92641000	-2.72136100	-1.47585200
P	-0.92639900	-2.72145700	1.47578700
P	-0.89253000	0.78753500	-2.43256900
P	-3.41738900	1.56435200	0.00001300
P	-0.99741600	3.15989700	0.00005600
P	-0.89252700	0.78742700	2.43256400
P	1.55237100	-0.75084200	2.73561200
P	2.02887000	2.44667400	1.48250300
P	2.02886900	2.44672700	-1.48241600
Zn	-3.28994100	-0.66161900	-0.00000100

B₁₂P₁₂-Zn (M2)

Symbol	X	Y	Z
B	-0.49657900	-0.52326300	2.41012100
B	1.66089800	-2.18172400	1.18212100
B	1.63559100	0.52647800	2.43084000
B	-0.50667400	2.16912500	1.18230200
B	3.28309700	0.01925800	-0.00039800
B	2.21789800	2.14656100	0.00115600
B	1.63468300	0.52970300	-2.43050100
B	-0.50699700	2.17078200	-1.17909300
B	1.66052300	-2.18013200	-1.18541100
B	-0.49734400	-0.51995300	-2.41053200
B	-2.39466200	-0.00747000	0.00048600
B	-1.06560800	-2.12759500	-0.00103100
P	3.11103200	1.26214400	1.46662700
P	3.11042800	1.26398600	-1.46569300
P	3.15613100	-1.88831400	-0.00168200
P	1.21681200	-1.31466000	2.82294100
P	-0.08164800	1.31054300	2.83142400
P	0.52416400	-3.19513200	-0.00212300
P	-1.95977100	-1.27082200	1.46482600
P	-1.96014000	-1.26886200	-1.46554300
P	-1.99261100	1.89651300	0.00170200
P	0.62316700	3.19897400	0.00207200
P	-0.08252400	1.31438300	-2.82950500
P	1.21589100	-1.31094400	-2.82497400
Zn	-4.54460300	-0.00253200	-0.00004600

B₁₂P₁₂-Zn (M3)

Symbol	X	Y	Z
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B	0.36433900	-2.78887700	0.02641800
B	2.82438600	-1.19956300	-0.62873300
B	1.36179500	-1.67586000	1.89501600
B	-1.65768000	-1.10213500	1.35546900
B	2.58853800	1.00174000	1.39007900
B	0.46292400	1.08022500	2.27706300
B	0.68948100	2.85727000	-0.06665500
B	-2.09286800	1.77325400	0.57532600
B	2.43997100	0.93287900	-1.57499300
B	-0.49827300	1.77281400	-1.69449200
B	-1.75615400	-1.37103600	-1.17902800
B	0.46864300	-1.12577600	-2.31875700
P	1.88252700	-0.09029300	2.81419500
P	1.49787100	2.57118600	1.64079200
P	3.62991800	0.48528300	-0.13116500
P	2.24134900	-2.63881700	0.48637100
P	-0.38184000	-2.49227900	1.78519800
P	2.33893800	-0.77895400	-2.45290300
P	-0.44908000	-2.72008200	-1.70214900
P	-1.03600200	0.05119800	-2.33152600
P	-3.09826400	-1.72021700	0.16322200
P	-1.37248900	0.71606200	1.96849300
P	-1.19436800	3.07602700	-0.45579700
P	1.31776200	2.45892800	-1.81918500
Zn	-3.55401200	0.51515500	0.00777500

B₁₂P₁₂-Zn (M4)

Symbol	X	Y	Z
B	-0.14256600	-2.35320400	1.22612300

B	-2.84588900	-1.09960700	1.20985300
B	-1.24229800	-2.50066800	-0.87547300
B	1.45938400	-1.26502400	-1.03486600
B	-2.86809300	-0.11072100	-1.60046000
B	-0.76212200	-0.19462500	-2.70140500
B	-1.23191200	2.35203700	-1.22525300
B	1.46471800	1.09446200	-1.20541400
B	-2.84038900	1.27085500	1.03853200
B	-0.13202800	2.50208400	0.87611400
B	1.48910200	0.11054000	1.59769500
B	-0.61029600	0.19440400	2.69887600
P	-2.00418000	-1.63978200	-2.40014400
P	-1.99767800	1.28420700	-2.61076400
P	-3.88001400	0.00795000	0.01496400
P	-1.99270000	-2.77594000	0.88083300
P	0.60694000	-2.87850300	-0.47256300
P	-2.51766800	0.19188000	2.60543800
P	0.62536300	-1.28528800	2.61084500
P	0.63180000	1.64082000	2.40010200
P	2.49605900	-0.00766800	-0.01322000
P	1.14742900	-0.19200600	-2.60719100
P	0.61913400	2.77536200	-0.88016900
P	-1.98044000	2.87918700	0.47313600
Zn	5.50004200	-0.00019800	-0.00135400

B₁₂P₁₂-Zn-SO₂ (N1)

Symbol	X	Y	Z
B	1.75738400	-1.49929800	0.31003100
B	-0.47673300	-0.81788900	2.31892600

B	-0.39464600	-2.73599800	0.12186100
B	-0.02323100	-0.92252400	-2.12939700
B	-3.01760600	-1.74799400	1.01408200
B	-2.78071900	-1.80097100	-1.32006800
B	-3.78461700	0.82554900	-0.30083200
B	-1.74316700	0.76733600	-2.41320300
B	-2.21139200	0.87267400	2.18049400
B	-2.21792300	2.59971500	-0.18203100
B	0.68817900	2.04990800	-0.94974600
B	0.47110300	2.10217100	1.18133200
P	-2.24075200	-3.15051100	-0.05498100
P	-4.22611100	-1.02979300	-0.30425300
P	-2.38918000	-0.98929900	2.65314100
P	0.63118000	-2.24324400	1.69068700
P	0.92924900	-2.31574700	-1.23066600
P	-0.35100400	1.08930600	2.59837900
P	2.13531100	2.04068900	0.27576200
P	-0.45253200	3.29513900	-0.01884300
P	0.16378700	0.97207000	-2.45652300
P	-1.83199300	-1.11369100	-2.83142400
P	-3.11275100	1.92288500	-1.74359000
P	-3.41222100	1.99022000	1.19666400
Zn	3.13166200	-0.04995100	0.42847200
S	6.23566100	-0.16542200	-0.14803500
O	5.04127500	-0.06476900	0.79291200
O	5.87143300	-0.10254300	-1.57518000

B₁₂P₁₂-Zn-SO₂ (N₂)

Symbol X Y Z

B	-0.13507700	-0.01019200	2.46383300
B	-1.68162700	2.31021400	1.39708600
B	-2.47421900	-0.40719100	2.34218800
B	-0.83171000	-2.45611200	0.95042600
B	-3.80639500	0.79202800	-0.03732900
B	-3.38703800	-1.53698300	-0.25703700
B	-2.27173600	0.08439300	-2.49221900
B	-0.73559200	-2.21882400	-1.41321800
B	-1.58196700	2.54831600	-0.95658500
B	0.06547400	0.47565700	-2.33904900
B	1.58248000	-0.77000800	0.02593800
B	0.97377400	1.61815800	0.24844600
P	-4.05500600	-0.59057900	1.28673000
P	-3.93236000	-0.29352600	-1.62815500
P	-3.14744500	2.57366100	0.17098000
P	-1.57167400	1.18877700	2.93840000
P	-1.06542300	-1.68458600	2.67748100
P	-0.25935900	3.07791500	0.34412800
P	1.51866800	0.39032700	1.62298700
P	1.63477400	0.68723100	-1.29327100
P	0.71709500	-2.49209700	-0.18559300
P	-2.15172100	-2.99195900	-0.35308100
P	-0.83116200	-1.11270100	-2.96222800
P	-1.33555200	1.75970200	-2.67777900
Zn	3.68425400	-1.36711200	0.05560200
S	5.54465400	0.78406600	0.31111500
O	4.58449700	1.85861700	0.00292300
O	6.58594900	0.47120400	-0.68008200

B₁₂P₁₂-Zn-SO₂ (N3)

Symbol	X	Y	Z
B	0.36433900	-2.78887700	0.02641800
B	2.82438600	-1.19956300	-0.62873300
B	1.36179500	-1.67586000	1.89501600
B	-1.65768000	-1.10213500	1.35546900
B	2.58853800	1.00174000	1.39007900
B	0.46292400	1.08022500	2.27706300
B	0.68948100	2.85727000	-0.06665500
B	-2.09286800	1.77325400	0.57532600
B	2.43997100	0.93287900	-1.57499300
B	-0.49827300	1.77281400	-1.69449200
B	-1.75615400	-1.37103600	-1.17902800
B	0.46864300	-1.12577600	-2.31875700
P	1.88252700	-0.09029300	2.81419500
P	1.49787100	2.57118600	1.64079200
P	3.62991800	0.48528300	-0.13116500
P	2.24134900	-2.63881700	0.48637100
P	-0.38184000	-2.49227900	1.78519800
P	2.33893800	-0.77895400	-2.45290300
P	-0.44908000	-2.72008200	-1.70214900
P	-1.03600200	0.05119800	-2.33152600
P	-3.09826400	-1.72021700	0.16322200
P	-1.37248900	0.71606200	1.96849300
P	-1.19436800	3.07602700	-0.45579700
P	1.31776200	2.45892800	-1.81918500
Zn	-3.55401200	0.51515500	0.00777500
S	-8.00222414	0.41632391	0.02530978

O	-8.89180622	-0.73733978	-0.11644837
O	-8.58181117	1.75876087	0.09113864

B₁₂P₁₂-Zn-SO₂ (N4)

Symbol	X	Y	Z
B	-0.14256600	-2.35320400	1.22612300
B	-2.84588900	-1.09960700	1.20985300
B	-1.24229800	-2.50066800	-0.87547300
B	1.45938400	-1.26502400	-1.03486600
B	-2.86809300	-0.11072100	-1.60046000
B	-0.76212200	-0.19462500	-2.70140500
B	-1.23191200	2.35203700	-1.22525300
B	1.46471800	1.09446200	-1.20541400
B	-2.84038900	1.27085500	1.03853200
B	-0.13202800	2.50208400	0.87611400
B	1.48910200	0.11054000	1.59769500
B	-0.61029600	0.19440400	2.69887600
P	-2.00418000	-1.63978200	-2.40014400
P	-1.99767800	1.28420700	-2.61076400
P	-3.88001400	0.00795000	0.01496400
P	-1.99270000	-2.77594000	0.88083300
P	0.60694000	-2.87850300	-0.47256300
P	-2.51766800	0.19188000	2.60543800
P	0.62536300	-1.28528800	2.61084500
P	0.63180000	1.64082000	2.40010200
P	2.49605900	-0.00766800	-0.01322000
P	1.14742900	-0.19200600	-2.60719100
P	0.61913400	2.77536200	-0.88016900
P	-1.98044000	2.87918700	0.47313600

Zn	5.50004200	-0.00019800	-0.00135400
S	7.89681300	-0.01917965	-0.40398505
O	8.62174034	1.24610343	-0.27776833
O	8.65426059	-1.26018369	-0.57302257