**Quantum Mechanics Approach for Metal-Organic Frameworks Deformation Effect on Carbon Capture Performance: A Density Functional Theory Study**

**Crystallographic Information File (CIF) hMOF-13**

data\_functionalizedCrystal

\_audit\_creation\_method 'MofGen! by Chris Wilmer'

\_symmetry\_space\_group\_name\_H-M 'P1'

\_symmetry\_Int\_Tables\_number 1

\_symmetry\_cell\_setting triclinic

loop\_

\_symmetry\_equiv\_pos\_as\_xyz

 x,y,z

\_cell\_length\_a 12.759401

\_cell\_length\_b 12.759400

\_cell\_length\_c 12.759393

\_cell\_angle\_alpha 89.970195

\_cell\_angle\_beta 89.980198

\_cell\_angle\_gamma 90.013730

loop\_

\_atom\_site\_label

\_atom\_site\_type\_symbol

\_atom\_site\_fract\_x

\_atom\_site\_fract\_y

\_atom\_site\_fract\_z

Zn1 Zn 1.606267 -0.418241 -0.593993

Zn2 Zn 2.106267 0.081759 -0.093993

Zn3 Zn 1.606158 -0.593957 -0.418316

Zn4 Zn 2.106158 -0.093957 0.081684

Zn5 Zn 1.430565 -0.418290 -0.418332

Zn6 Zn 1.930565 0.081710 0.081668

Zn7 Zn 1.430558 -0.593876 -0.593956

Zn8 Zn 1.930558 -0.093876 -0.093956

O9 O 1.518387 -0.506091 -0.506149

O10 O 2.018387 -0.006091 -0.006149

O11 O 1.753273 -0.441564 -0.570698

O12 O 2.253273 0.058436 -0.070698

O13 O 1.582823 -0.570708 -0.271297

O14 O 2.082823 -0.070708 0.228703

O15 O 1.453921 -0.271262 -0.441656

O16 O 1.953921 0.228738 0.058344

O17 O 1.753193 -0.570661 -0.441628

O18 O 2.253193 -0.070661 0.058372

O19 O 1.583008 -0.271226 -0.570714

O20 O 2.083008 0.228774 -0.070714

O21 O 1.453816 -0.441646 -0.271309

O22 O 1.953816 0.058354 0.228691

O23 O 1.283543 -0.441568 -0.441620

O24 O 1.783543 0.058432 0.058380

O25 O 1.453908 -0.570523 -0.740982

O26 O 1.953908 -0.070523 -0.240982

O27 O 1.283538 -0.570570 -0.570651

O28 O 1.783538 -0.070570 -0.070651

O29 O 1.583001 -0.441485 -0.741009

O30 O 2.083001 0.058515 -0.241009

O31 O 1.582815 -0.740967 -0.441592

O32 O 2.082815 -0.240967 0.058408

O33 O 1.453802 -0.740908 -0.570635

O34 O 1.953802 -0.240908 -0.070635

C35 C 1.245420 -0.506066 -0.506134

C36 C 1.745420 -0.006066 -0.006134

C37 C 1.128643 -0.506081 -0.506152

C38 C 1.628643 -0.006081 -0.006152

C39 C 0.964086 -0.439006 -0.573470

C40 C 1.464086 0.060994 -0.073470

C41 C 1.073810 -0.438985 -0.573463

C42 C 1.573810 0.061015 -0.073463

C43 C 1.073746 -0.573210 -0.438852

C44 C 1.573746 -0.073210 0.061148

C45 C 0.964024 -0.573235 -0.438865

C46 C 1.464024 -0.073235 0.061135

C47 C 1.518325 -0.779058 -0.506131

C48 C 2.018325 -0.279058 -0.006131

C49 C 1.518394 -0.895835 -0.506158

C50 C 2.018394 -0.395835 -0.006158

C51 C 1.585581 -0.950588 -0.573415

C52 C 2.085581 -0.450588 -0.073415

C53 C 1.585640 -1.060312 -0.573444

C54 C 2.085640 -0.560312 -0.073444

C55 C 1.451323 -1.060520 -0.438948

C56 C 1.951323 -0.560520 0.061052

C57 C 1.451260 -0.950798 -0.438926

C58 C 1.951260 -0.450798 0.061074

C59 C 1.792420 -0.506116 -0.506165

C60 C 2.292420 -0.006116 -0.006165

C61 C 1.909197 -0.506127 -0.506172

C62 C 2.409197 -0.006127 -0.006172

C63 C 1.518466 -0.505990 -0.780183

C64 C 2.018466 -0.005990 -0.280183

C65 C 1.518499 -0.505947 -0.896959

C66 C 2.018499 -0.005947 -0.396959

C67 C 1.518478 -0.232057 -0.506191

C68 C 2.018478 0.267943 -0.006191

C69 C 1.518517 -0.115281 -0.506209

C70 C 2.018517 0.384719 -0.006209

C71 C 1.585723 -0.438746 -0.951837

C72 C 2.085723 0.061254 -0.451837

C73 C 1.585740 -0.438701 -1.061561

C74 C 2.085740 0.061299 -0.561561

C75 C 1.451308 -0.573066 -1.061520

C76 C 1.951308 -0.073066 -0.561520

C77 C 1.451286 -0.573105 -0.951798

C78 C 1.951286 -0.073105 -0.451798

C79 C 1.518369 -0.506115 -0.233182

C80 C 2.018369 -0.006115 0.266818

C81 C 1.518539 -0.505862 -0.116406

C82 C 2.018539 -0.005862 0.383594

H83 H 1.118496 -0.384330 -0.628264

H84 H 1.618496 0.115670 -0.128264

H85 H 1.640244 -0.905840 -0.628161

H86 H 2.140244 -0.405840 -0.128161

H87 H 1.118400 -0.627844 -0.384050

H88 H 1.618400 -0.127844 0.115950

H89 H 1.396666 -1.105284 -0.384209

H90 H 1.896666 -0.605284 0.115791

H91 H 0.919449 -0.384362 -0.628276

H92 H 1.419449 0.115638 -0.128276

H93 H 1.396588 -0.627747 -1.106183

H94 H 1.896588 -0.127747 -0.606183

H95 H 0.919332 -0.627899 -0.384062

H96 H 1.419332 -0.127899 0.115938

H97 H 1.640347 -1.104888 -0.628214

H98 H 2.140347 -0.604888 -0.128214

F99 F 1.379740 -0.892521 -0.367344

F100 F 1.879740 -0.392521 0.132656

H101 H 1.640449 -0.384058 -0.907191

H102 H 2.140449 0.115942 -0.407191

H103 H 1.640479 -0.383977 -1.106238

H104 H 2.140479 0.116023 -0.606238

F105 F 1.379728 -0.644629 -0.893390

F106 F 1.879728 -0.144629 -0.393390

**Setup and Parameters BFGS Simulation**

&CONTROL

 calculation = 'relax',

 restart\_mode = 'from\_scratch',

 prefix = 'hMOF\_13\_md',

 pseudo\_dir = './pseudo',

 outdir = './output\_md/',

 tprnfor = .true.,

 tstress = .true.,

 nstep = 1000,

 dt = 1.0,

 disk\_io = 'low'

/

&SYSTEM

 ibrav = 0,

 nat = 106,

 ntyp = 5,

 ecutwfc = 50.0,

 ecutrho = 200.0,

 occupations = 'smearing',

 smearing = 'gaussian',

 degauss = 0.05,

 input\_dft = 'PBE',

 nspin = 4

/

&ELECTRONS

 conv\_thr = 1.0d-6,

 mixing\_beta = 0.7,

 diagonalization = 'david',

 electron\_maxstep = 100

/

&IONS

 ion\_dynamics = 'bfgs',

 ion\_temperature = 'rescaling',

 tempw = 305.0,

 tolp = 100

/

&CELL

 cell\_dynamics = 'pr',

 press = 1.0,

 cell\_dofree = 'all'

 wmass = 125.67

/

CELL\_PARAMETERS {angstrom}

 12.759401 0.000000 0.000000

 -0.003050 12.759399 0.000000

 0.004466 0.006673 12.759391

ATOMIC\_SPECIES

 Zn 65.38 Zn.pbe-dnl-kjpaw\_psl.1.0.0.UPF

 O 15.999 O.pbe-n-kjpaw\_psl.1.0.0.UPF

 C 12.011 C.pbe-n-kjpaw\_psl.1.0.0.UPF

 H 1.008 H.pbe-kjpaw\_psl.1.0.0.UPF

 F 18.998 F.pbe-n-kjpaw\_psl.1.0.0.UPF

ATOMIC\_POSITIONS (crystal)

Zn 1.606267 -0.418241 -0.593993

Zn 2.106267 0.081759 -0.093993

Zn 1.606158 -0.593957 -0.418316

Zn 2.106158 -0.093957 0.081684

Zn 1.430565 -0.418290 -0.418332

Zn 1.930565 0.081710 0.081668

Zn 1.430558 -0.593876 -0.593956

Zn 1.930558 -0.093876 -0.093956

O 1.518387 -0.506091 -0.506149

O 2.018387 -0.006091 -0.006149

O 1.753273 -0.441564 -0.570698

O 2.253273 0.058436 -0.070698

O 1.582823 -0.570708 -0.271297

O 2.082823 -0.070708 0.228703

O 1.453921 -0.271262 -0.441656

O 1.953921 0.228738 0.058344

O 1.753193 -0.570661 -0.441628

O 2.253193 -0.070661 0.058372

O 1.583008 -0.271226 -0.570714

O 2.083008 0.228774 -0.070714

O 1.453816 -0.441646 -0.271309

O 1.953816 0.058354 0.228691

O 1.283543 -0.441568 -0.441620

O 1.783543 0.058432 0.058380

O 1.453908 -0.570523 -0.740982

O 1.953908 -0.070523 -0.240982

O 1.283538 -0.570570 -0.570651

O 1.783538 -0.070570 -0.070651

O 1.583001 -0.441485 -0.741009

O 2.083001 0.058515 -0.241009

O 1.582815 -0.740967 -0.441592

O 2.082815 -0.240967 0.058408

O 1.453802 -0.740908 -0.570635

O 1.953802 -0.240908 -0.070635

C 1.245420 -0.506066 -0.506134

C 1.745420 -0.006066 -0.006134

C 1.128643 -0.506081 -0.506152

C 1.628643 -0.006081 -0.006152

C 0.964086 -0.439006 -0.573470

C 1.464086 0.060994 -0.073470

C 1.073810 -0.438985 -0.573463

C 1.573810 0.061015 -0.073463

C 1.073746 -0.573210 -0.438852

C 1.573746 -0.073210 0.061148

C 0.964024 -0.573235 -0.438865

C 1.464024 -0.073235 0.061135

C 1.518325 -0.779058 -0.506131

C 2.018325 -0.279058 -0.006131

C 1.518394 -0.895835 -0.506158

C 2.018394 -0.395835 -0.006158

C 1.585581 -0.950588 -0.573415

C 2.085581 -0.450588 -0.073415

C 1.585640 -1.060312 -0.573444

C 2.085640 -0.560312 -0.073444

C 1.451323 -1.060520 -0.438948

C 1.951323 -0.560520 0.061052

C 1.451260 -0.950798 -0.438926

C 1.951260 -0.450798 0.061074

C 1.792420 -0.506116 -0.506165

C 2.292420 -0.006116 -0.006165

C 1.909197 -0.506127 -0.506172

C 2.409197 -0.006127 -0.006172

C 1.518466 -0.505990 -0.780183

C 2.018466 -0.005990 -0.280183

C 1.518499 -0.505947 -0.896959

C 2.018499 -0.005947 -0.396959

C 1.518478 -0.232057 -0.506191

C 2.018478 0.267943 -0.006191

C 1.518517 -0.115281 -0.506209

C 2.018517 0.384719 -0.006209

C 1.585723 -0.438746 -0.951837

C 2.085723 0.061254 -0.451837

C 1.585740 -0.438701 -1.061561

C 2.085740 0.061299 -0.561561

C 1.451308 -0.573066 -1.061520

C 1.951308 -0.073066 -0.561520

C 1.451286 -0.573105 -0.951798

C 1.951286 -0.073105 -0.451798

C 1.518369 -0.506115 -0.233182

C 2.018369 -0.006115 0.266818

C 1.518539 -0.505862 -0.116406

C 2.018539 -0.005862 0.383594

H 1.118496 -0.384330 -0.628264

H 1.618496 0.115670 -0.128264

H 1.640244 -0.905840 -0.628161

H 2.140244 -0.405840 -0.128161

H 1.118400 -0.627844 -0.384050

H 1.618400 -0.127844 0.115950

H 1.396666 -1.105284 -0.384209

H 1.896666 -0.605284 0.115791

H 0.919449 -0.384362 -0.628276

H 1.419449 0.115638 -0.128276

H 1.396588 -0.627747 -1.106183

H 1.896588 -0.127747 -0.606183

H 0.919332 -0.627899 -0.384062

H 1.419332 -0.127899 0.115938

H 1.640347 -1.104888 -0.628214

H 2.140347 -0.604888 -0.128214

F 1.379740 -0.892521 -0.367344

F 1.879740 -0.392521 0.132656

H 1.640449 -0.384058 -0.907191

H 2.140449 0.115942 -0.407191

H 1.640479 -0.383977 -1.106238

H 2.140479 0.116023 -0.606238

F 1.379728 -0.644629 -0.893390

F 1.879728 -0.144629 -0.393390

K\_POINTS automatic

1 1 1 0 0 0

**Setup and Parameters DFT Simulation**

&CONTROL

 calculation = 'scf',

 restart\_mode = 'from\_scratch',

 prefix = 'hMOF\_13\_md',

 pseudo\_dir = './pseudo',

 outdir = './output\_md/',

 tprnfor = .true.,

 tstress = .true.,

 nstep = 1000,

 dt = 1.0,

 disk\_io = 'low'

/

&SYSTEM

 ibrav = 0,

 nat = 106,

 ntyp = 5,

 ecutwfc = 50.0,

 ecutrho = 200.0,

 occupations = 'smearing',

 smearing = 'gaussian',

 degauss = 0.05,

 input\_dft = 'PBE',

 nspin = 4

/

&ELECTRONS

 conv\_thr = 1.0d-6,

 mixing\_beta = 0.7,

 diagonalization = 'david',

 electron\_maxstep = 100

/

&IONS

 ion\_dynamics = 'beeman',

 ion\_temperature = 'rescaling',

 tempw = 305.0,

 tolp = 100

/

&CELL

 cell\_dynamics = 'pr',

 press = 1.0,

 cell\_dofree = 'all'

 wmass = 125.67

/

CELL\_PARAMETERS {angstrom}

 12.759401 0.000000 0.000000

 -0.003050 12.759399 0.000000

 0.004466 0.006673 12.759391

ATOMIC\_SPECIES

 Zn 65.38 Zn.pbe-dnl-kjpaw\_psl.1.0.0.UPF

 O 15.999 O.pbe-n-kjpaw\_psl.1.0.0.UPF

 C 12.011 C.pbe-n-kjpaw\_psl.1.0.0.UPF

 H 1.008 H.pbe-kjpaw\_psl.1.0.0.UPF

 F 18.998 F.pbe-n-kjpaw\_psl.1.0.0.UPF

ATOMIC\_POSITIONS (crystal)

Zn 1.606267 -0.418241 -0.593993

Zn 2.106267 0.081759 -0.093993

Zn 1.606158 -0.593957 -0.418316

Zn 2.106158 -0.093957 0.081684

Zn 1.430565 -0.418290 -0.418332

Zn 1.930565 0.081710 0.081668

Zn 1.430558 -0.593876 -0.593956

Zn 1.930558 -0.093876 -0.093956

O 1.518387 -0.506091 -0.506149

O 2.018387 -0.006091 -0.006149

O 1.753273 -0.441564 -0.570698

O 2.253273 0.058436 -0.070698

O 1.582823 -0.570708 -0.271297

O 2.082823 -0.070708 0.228703

O 1.453921 -0.271262 -0.441656

O 1.953921 0.228738 0.058344

O 1.753193 -0.570661 -0.441628

O 2.253193 -0.070661 0.058372

O 1.583008 -0.271226 -0.570714

O 2.083008 0.228774 -0.070714

O 1.453816 -0.441646 -0.271309

O 1.953816 0.058354 0.228691

O 1.283543 -0.441568 -0.441620

O 1.783543 0.058432 0.058380

O 1.453908 -0.570523 -0.740982

O 1.953908 -0.070523 -0.240982

O 1.283538 -0.570570 -0.570651

O 1.783538 -0.070570 -0.070651

O 1.583001 -0.441485 -0.741009

O 2.083001 0.058515 -0.241009

O 1.582815 -0.740967 -0.441592

O 2.082815 -0.240967 0.058408

O 1.453802 -0.740908 -0.570635

O 1.953802 -0.240908 -0.070635

C 1.245420 -0.506066 -0.506134

C 1.745420 -0.006066 -0.006134

C 1.128643 -0.506081 -0.506152

C 1.628643 -0.006081 -0.006152

C 0.964086 -0.439006 -0.573470

C 1.464086 0.060994 -0.073470

C 1.073810 -0.438985 -0.573463

C 1.573810 0.061015 -0.073463

C 1.073746 -0.573210 -0.438852

C 1.573746 -0.073210 0.061148

C 0.964024 -0.573235 -0.438865

C 1.464024 -0.073235 0.061135

C 1.518325 -0.779058 -0.506131

C 2.018325 -0.279058 -0.006131

C 1.518394 -0.895835 -0.506158

C 2.018394 -0.395835 -0.006158

C 1.585581 -0.950588 -0.573415

C 2.085581 -0.450588 -0.073415

C 1.585640 -1.060312 -0.573444

C 2.085640 -0.560312 -0.073444

C 1.451323 -1.060520 -0.438948

C 1.951323 -0.560520 0.061052

C 1.451260 -0.950798 -0.438926

C 1.951260 -0.450798 0.061074

C 1.792420 -0.506116 -0.506165

C 2.292420 -0.006116 -0.006165

C 1.909197 -0.506127 -0.506172

C 2.409197 -0.006127 -0.006172

C 1.518466 -0.505990 -0.780183

C 2.018466 -0.005990 -0.280183

C 1.518499 -0.505947 -0.896959

C 2.018499 -0.005947 -0.396959

C 1.518478 -0.232057 -0.506191

C 2.018478 0.267943 -0.006191

C 1.518517 -0.115281 -0.506209

C 2.018517 0.384719 -0.006209

C 1.585723 -0.438746 -0.951837

C 2.085723 0.061254 -0.451837

C 1.585740 -0.438701 -1.061561

C 2.085740 0.061299 -0.561561

C 1.451308 -0.573066 -1.061520

C 1.951308 -0.073066 -0.561520

C 1.451286 -0.573105 -0.951798

C 1.951286 -0.073105 -0.451798

C 1.518369 -0.506115 -0.233182

C 2.018369 -0.006115 0.266818

C 1.518539 -0.505862 -0.116406

C 2.018539 -0.005862 0.383594

H 1.118496 -0.384330 -0.628264

H 1.618496 0.115670 -0.128264

H 1.640244 -0.905840 -0.628161

H 2.140244 -0.405840 -0.128161

H 1.118400 -0.627844 -0.384050

H 1.618400 -0.127844 0.115950

H 1.396666 -1.105284 -0.384209

H 1.896666 -0.605284 0.115791

H 0.919449 -0.384362 -0.628276

H 1.419449 0.115638 -0.128276

H 1.396588 -0.627747 -1.106183

H 1.896588 -0.127747 -0.606183

H 0.919332 -0.627899 -0.384062

H 1.419332 -0.127899 0.115938

H 1.640347 -1.104888 -0.628214

H 2.140347 -0.604888 -0.128214

F 1.379740 -0.892521 -0.367344

F 1.879740 -0.392521 0.132656

H 1.640449 -0.384058 -0.907191

H 2.140449 0.115942 -0.407191

H 1.640479 -0.383977 -1.106238

H 2.140479 0.116023 -0.606238

F 1.379728 -0.644629 -0.893390

F 1.879728 -0.144629 -0.393390

K\_POINTS automatic

1 1 1 0 0 0