Přílohy

Příloha 1: vstupní kód Cu(111) - Cu(2p)

```
cluster surface off
cluster Rmax l(A) 15
cluster reference-point l(A) 0 0 0

add cluster layer Cu l(A) 0 0 0 2.55266 2.55266 30 60
add cluster layer Cu l(A) 1.4737763 0 -2.0842345 2.55266 2.55266 30 60
add cluster layer Cu l(A) 2.9475527 0 -4.1684690 2.55266 2.55266 30 60
add cluster layer Cu l(A) 0 0 -6.2527034 2.55276 2.55266 30 60
add cluster layer Cu l(A) 1.4737763 0 -8.3369379 2.55266 2.55266 30 60
add cluster layer Cu l(A) 2.9475527 0 -10.421172 2.55266 2.55266 30 60
add cluster layer Cu l(A) 0 0 -12.505407 2.55266 2.55266 30 60

rotate cluster z -30

cluster natoms 250

cluster output l(A) data.cls

emitters 3 l(A)  1.276328 -0.736881 -2.08423447 0
1.2763257 0.73689204 -4.168469 0
0.0 0.0 -6.252703 0

movable cluster
beta 68
emission energy E(eV) 530 530 1
emission angle theta 0 70 71
emission angle phi 0 360 361
polarization LPx

initial state 2p3/2

V0 E(eV) 11

imfp inline 1 l(A) 10

lmax 12

iteration recursion
orders 1 10
muffin-tin

emission angle window 4

temperature 300 345
scan pd output2.dat

time
end
```

Příloha 2: vstupní kód CeO_2(111) - Ce(3d)

```
cluster surface off
cluster Rmax l(A) 20
cluster reference-point l(A) 0 0 0

add cluster layer O l(A) 2.20902 0 0 3.826 3.826 30 60
add cluster layer Ce l(A) 0 0 -0.781 3.826 3.826 30 60
add cluster layer O l(A) -2.20902 0 -1.562 3.826 3.826 30 60

add cluster layer O l(A) 0 0 -3.124 3.826 3.826 30 60
add cluster layer Ce l(A) -2.20902 0 -3.905 3.826 3.826 30 60
add cluster layer O l(A) 2.20902 0 -4.686 3.826 3.826 30 60

add cluster layer O l(A) -2.20902 0 -6.248 3.826 3.826 30 60
add cluster layer Ce l(A) 2.20902 0 -7.029 3.826 3.826 30 60
add cluster layer O l(A) 0 0 -7.81 3.826 3.826 30 60
```

```
16
17 add cluster layer O l(A) 2.20902 0 -9.372 3.826 3.826 30 60
18 add cluster layer Ce l(A) 0 0 -10.153 3.826 3.826 30 60
19 add cluster layer O l(A) -2.20902 0 -10.934 3.826 3.826 30 60
20
21 cluster natoms 300
22
23 rotate cluster z -30
24
25 emitters 4 l(A)
26 0 0 -0.781 0
27 0 -2.2090309 -3.9050002 4
28 0 2.2090309 -7.029 7
29 0 0 -10.153001 0
30
31 cluster output l(A) data.cls
32
33 movable cluster
34 beta 68
35 emission energy E(eV) 570 570 1
36 emission angle theta 0 70 71
37 emission angle phi 0 360 361
38 polarization LPx
39
40 initial state 3d3/2
41
42 V0 E(eV) 10.4
43
44 imfp inline 1 l(A) 11.81
45
46 lmax 12
47
48 iteration recursion
49 orders 1 10
50 muffin-tin
51
52 emission angle window 4
53
54 temperature 300 355
55
56 scan pd j541L
57
58 time
59 end
```

Příloha 3: vstupní kód $Ce_2O_3(111)$ - O(1s)

```
1  cluster surface on
2  cluster Rmax l(A) 25
3  cluster reference-point l(A) 0 0 44.466072
4
5  cluster input cluster.cls
6
7  cluster natoms 350
8
9  cluster output l(A) data.cls
10
11 emitters 8 l(A)
12 -0.096010000 2.192570000 45.570810000 3
13 2.18322 3.76375 47.01612 6
14 -1.94683 1.01314 43.36134 8
15 -3.81298 2.56755 45.32443 11
16 0.22107 -7.03376 47.1729 13
17 0.09601 7.12365 46.65512 15
18 -2.18322 -3.76376 41.91602 8
19 -2.08721 -0.94979006 40.585335 8
20
21 movable cluster
22 beta 68
23 emission energy E(eV) 957 957 1
24 emission angle theta 0 70 71
25 emission angle phi 0 360 361
26 polarization LPy
```

```
initial state 1s

V0 E(eV) 9.7

imfp inline 1 l(A) 17.16

lmax 12

iteration recursion
orders 1 10
muffin-tin

emission angle window 4

temperature 300 355

scan pd output2y.dat

time
end
```

Příloha 4: CIF soubor pro kubickou strukturu Ce_2O_3 (bixbyit)

```
data_DiceriumTrioxideC

_audit_creation_method                   'Crystallographica 2'
_cell_angle_alpha                        90
_cell_angle_beta                         90
_cell_angle_gamma                        90
_cell_formula_units_Z                    16
_cell_length_a                           11.41
_cell_length_b                           11.41
_cell_length_c                           11.41
_cell_volume                             1485.45
_cgraph_comments                         'Ab initio calculation of the
                                          crystal structure of the
                                          lanthanide Ln2O3 sesquioxide'
_cgraph_title                            'Dicerium Trioxide - C'
_chemical_formula_sum                    'Ce2 O3'
_symmetry_space_group_name_H-M           'I a -3'
_symmetry_space_group_name_Hall          '-I 2b 2c 3'

loop_
        _symmetry_equiv_pos_as_xyz
        'x, y, z'
        'x+1/2, y+1/2, z+1/2'
        '-x, -y, -z'
        '-x+1/2, -y+1/2, -z+1/2'
        'z, x, y'
        'z+1/2, x+1/2, y+1/2'
        '-z, -x, -y'
        '-z+1/2, -x+1/2, -y+1/2'
        'y, z, x'
        'y+1/2, z+1/2, x+1/2'
        '-y, -z, -x'
        '-y+1/2, -z+1/2, -x+1/2'
        '-y, -z+1/2, x'
        '-y+1/2, -z, x+1/2'
        'y, z+1/2, -x'
        'y+1/2, z, -x+1/2'
        'z, -x, -y+1/2'
        'z+1/2, -x+1/2, -y'
        '-z, x, y+1/2'
        '-z+1/2, x+1/2, y'
        '-y+1/2, z, -x'
        '-y, z+1/2, -x+1/2'
        'y+1/2, -z, x'
        'y, -z+1/2, x+1/2'
        '-z, -x+1/2, y'
        '-z+1/2, -x, y+1/2'
        'z, x+1/2, -y'
        'z+1/2, x, -y+1/2'
```

```
          '-z+1/2, x, -y'
          '-z, x+1/2, -y+1/2'
          'z+1/2, -x, y'
          'z, -x+1/2, y+1/2'
          'y, -z, -x+1/2'
          'y+1/2, -z+1/2, -x'
          '-y, z, x+1/2'
          '-y+1/2, z+1/2, x'
          '-x, -y+1/2, z'
          '-x+1/2, -y, z+1/2'
          'x, y+1/2, -z'
          'x+1/2, y, -z+1/2'
          'x, -y, -z+1/2'
          'x+1/2, -y+1/2, -z'
          '-x, y, z+1/2'
          '-x+1/2, y+1/2, z'
          '-x+1/2, y, -z'
          '-x, y+1/2, -z+1/2'
          'x+1/2, -y, z'
          'x, -y+1/2, z+1/2'

loop_
          _atom_site_label
          _atom_site_type_symbol
          _atom_site_fract_x
          _atom_site_fract_y
          _atom_site_fract_z
          _atom_site_U_iso_or_equiv
          _atom_site_thermal_displace_type
          _atom_site_occupancy
          Ce1 Ce3+ 0.25 0.25 0.25 0 Uiso 1
          Ce2 Ce3+ 0.9699 0 0.25 0 Uiso 1
          O1 O2- 0.3903 0.149 0.3784 0 Uiso 1

_eof
```