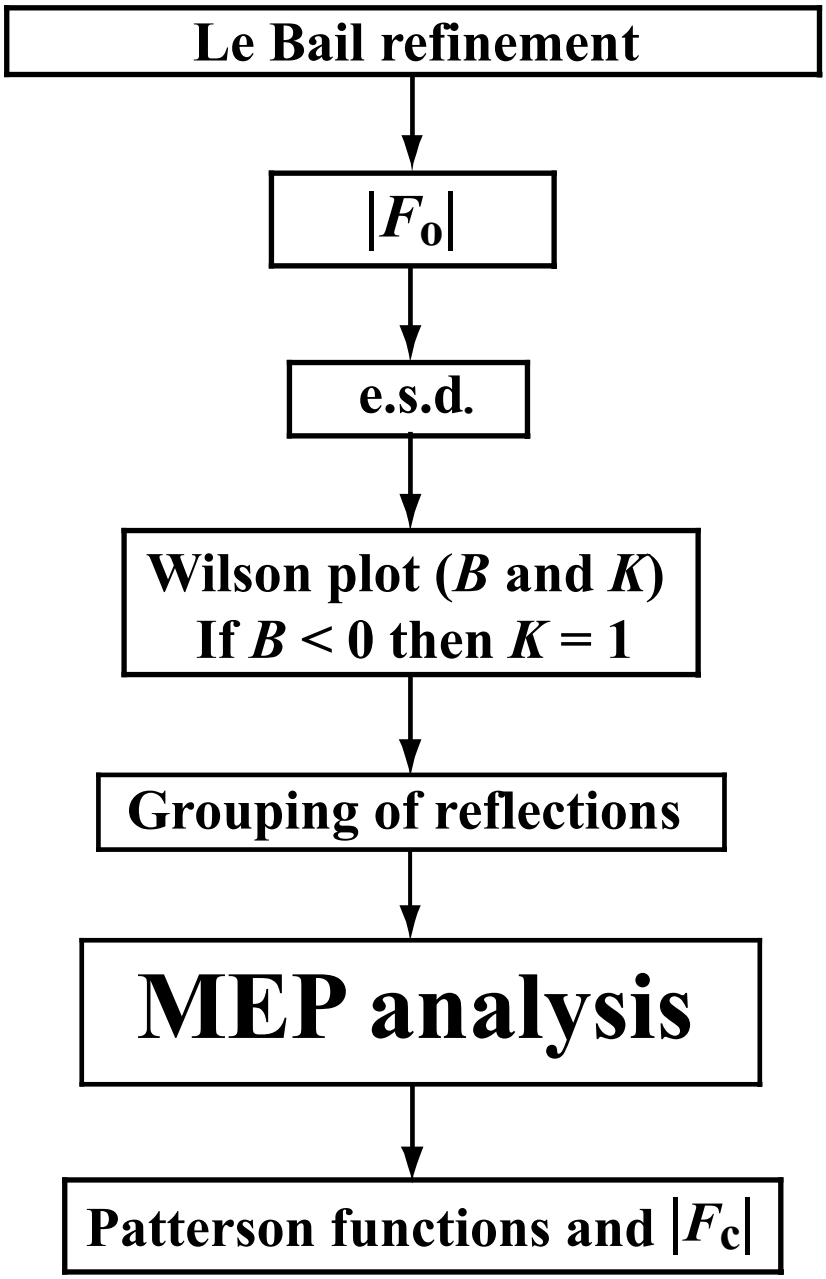
Appendix A. Flow chart of the maximum-entropy Patterson method



Appendix B. Examples

$BaSO_4$

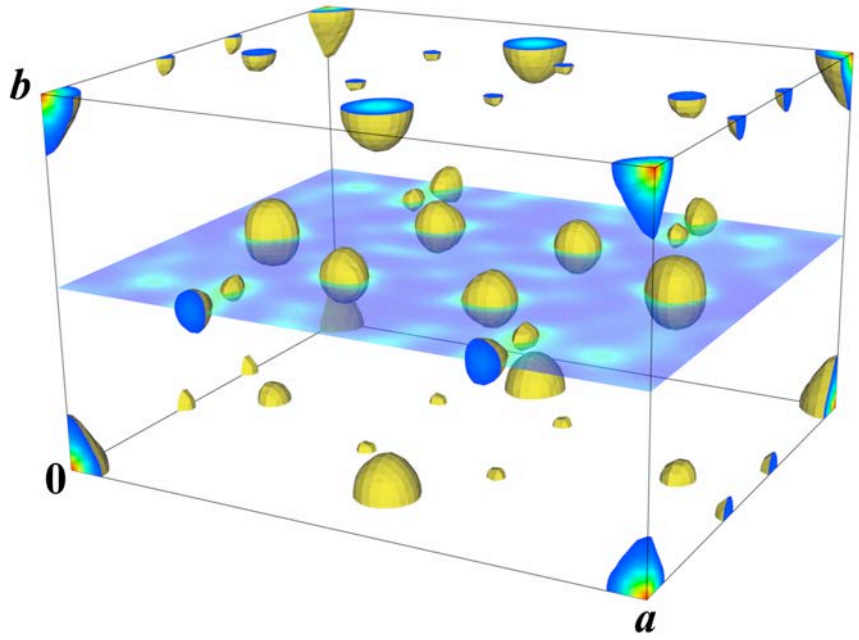
Crystal data

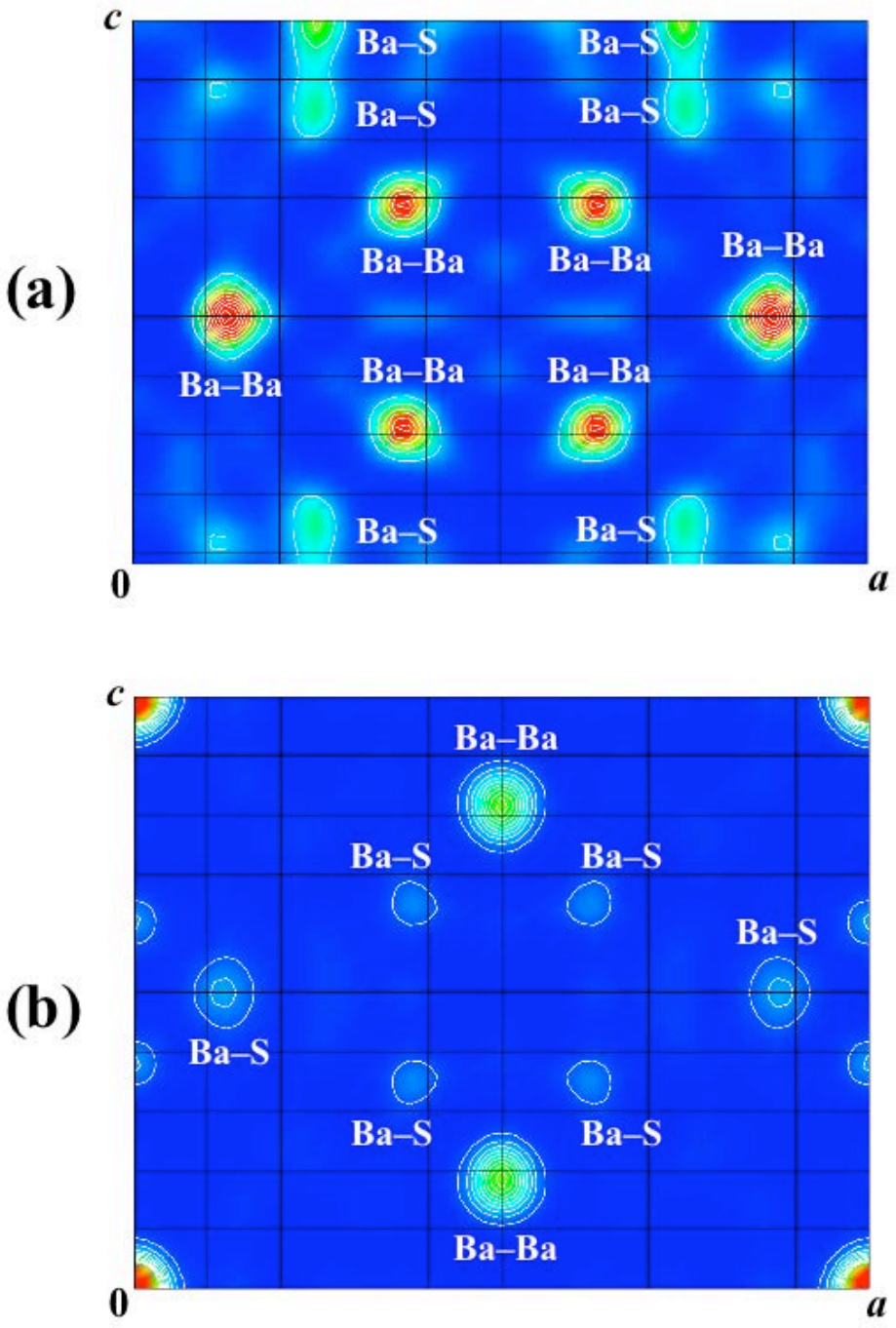
Symmetry	Orthorhombic
Space group number	62
Space group	*Pnma*
Patterson symmetry	*Pmmm*
a / Å	8.87590
b / Å	5.45213
c / Å	7.15271

Atoms	sites	*x*	*y*	*z*
Ba	4*c*	0.184409	1/4	0.158462
S	4*c*	0.062509	1/4	0.691072

Peaks positions for Patterson functions

Ba – Ba			Ba – S		
x	*y*	*z*	*x*	*y*	*z*
0	0	0	0.745	0	0.033
0.869	1/2	1/2	0.245	1/2	0.850
0.369	1/2	0.317	0.878	0	0.533
1/2	0	0.817	0.378	0	0.350





(0*k*0) Patterson map for $BaSO_4$
(a) $y = 1/2$ and (b) $y = 0$

Al_2O_3

Crystal data

Symmetry	Trigonal (hexagonal lattice)
Space group number	167
Space group	$R\bar{3}c$
Patterson symmetry	$R\bar{3}m$
a / Å	4.75737
c / Å	12.9871

+(0, 0, 0) (2/3, 1/3, 1/3) (2/3, 1/3, 1/3)

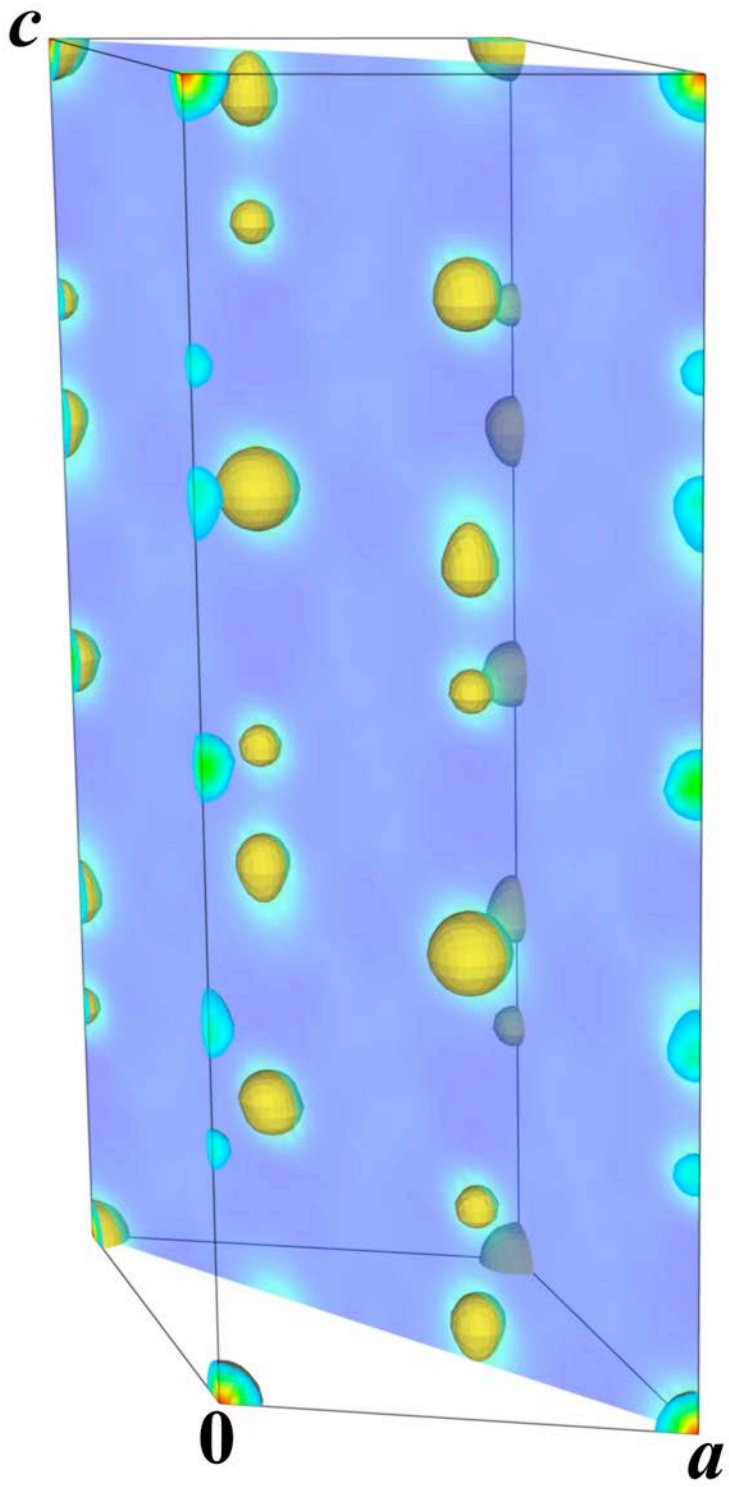
Atom	Site	*x*	*y*	*z*
Al	12*c*	0	0	0.35214
O	18*e*	0.30631	1/4	0.691072

Peaks positions for Patterson functions

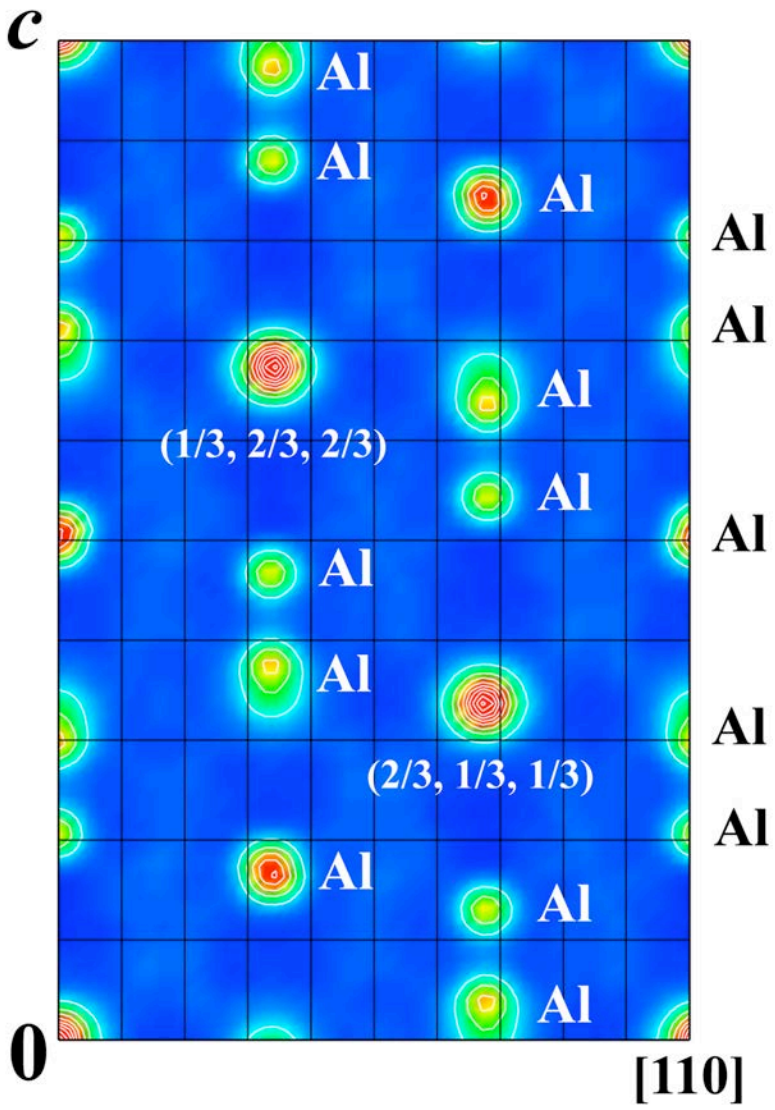
+(0, 0, 0) (2/3, 1/3, 1/3) (1/3, 2/3, 2/3)

Al – Al

x	*y*	*z*
0	0	0
0	0	0.204
0	0	0.296
0	0	0.704
0	0	0.796



Three-dimensional distribution of Patterson functions in the unit cell of Al_2O_3

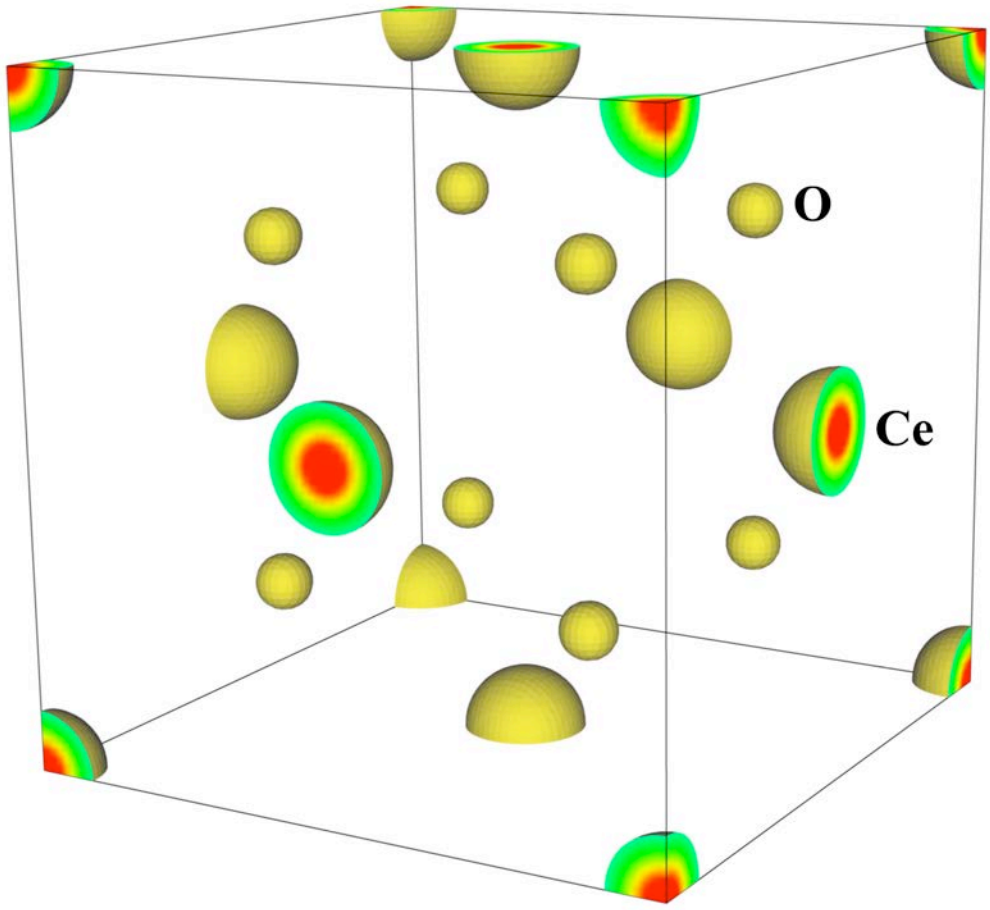


Patterson map of Al_2O_3 on the $(1\bar{1}00)$ plane

CeO_2

Crystal data	
Symmetry	Cubic
Space group number	225
Space group	$Fm\bar{3}m$
Patterson symmetry	$Fm\bar{3}m$
a / Å	5.41104

Atom	Site	x	y	z
Ce	4*a*	0	0	0
O	8*c*	1/4	1/4	1/4



Three-dimensional distribution of Patterson functions in the unit cell of CeO_2