

Supporting Information

Self-sacrificial template directed hydrothermal route to kesterite-Cu₂ZnSnS₄ microspheres and study of their photo response properties

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S1.

Crystallographic Information File (CIF)

data_CZTS microsphere (190 °C/24 h)

_audit_creation_date 'Mon Oct 12 15:11:53 PDT 1998'

_audit_creation_method 'Maud, version 2.33'

_audit_update_record 'Last update Tue Oct 22 18:48:20 IST 2013'

_computing_structure_refinement 'Maud, version 2.33'

_chemical_name_common 'kesterite'

_chemical_formula_sum 'Cu2 Zn Sn S4 '

_symmetry_cell_setting tetragonal

_symmetry_space_group_name_H-M I-42m

_symmetry_Int_Tables_number 121

_cell_formula_units_Z 1

_Chemical_formula_weight 439.471

loop_

_symmetry_equiv_pos_site_id

_symmetry_equiv_pos_as_xyz

1 x,y,z

2 1/2+x,1/2+y,1/2+z

3 -x,y,-z

4 -x,-y,z

5 x,-y,-z

6 1/2-x,1/2+y,1/2-z

7 1/2-x,1/2-y,1/2+z

8 $1/2+x, 1/2-y, 1/2-z$

9 $y, -x, -z$

10 $-y, x, -z$

11 $1/2+y, 1/2-x, 1/2-z$

12 $1/2-y, 1/2+x, 1/2-z$

13 $-y, -x, z$

14 y, x, z

15 $1/2-y, 1/2-x, 1/2+z$

16 $1/2+y, 1/2+x, 1/2+z$

_cell_length_a 5.424(1)

_cell_length_b 5.4238105

_cell_length_c 10.808(4)

_cell_angle_alpha 90

_cell_angle_beta 90

_cell_angle_gamma 90

_cell_volume 317.958

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_occupancy

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_B_iso_or_equiv

_atom_site_calc_flag

Cu(4d) Cu 0.5144217 0.0 0.5 0.25 1.0264388 .

Zn(4d) Zn 0.5136042 0.0 0.5 0.25 1.0264388 .

Cu(2a) Cu 1.0153217 0.0 0.0 0.0 1.1969856 .

Sn(2b) Sn 0.9242791 0.0 0.0 0.5 0.56138307 .

S(8i) S 0.9814857 0.75160086 0.75160086 0.884114 0.61191547 .
