

Supplementary Information

The effect of four-phonon scattering on the lattice thermal conductivity of Janus WSSe and WS₂ monolayers

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The structure files in the format of .cif for WSSe and WS₂ monolayers are given as follows:

WSSe:

```
data_created_by_vaspkit_code
_audit_creation_date          Wed Mar 11 17:33:42 2026
_pd_phase_name                'CIF files'
_cell_length_a                3.18402709
_cell_length_b                3.18402709
_cell_length_c                15.00000000
_cell_angle_alpha             90.0000
_cell_angle_beta              90.0000
_cell_angle_gamma             120.0000
_symmetry_space_group_name_H-M 'P 1'
_symmetry_Int_Tables_number   1
loop_
_symmetry_equiv_pos_as_xyz
  'x, y, z'
loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_thermal_displace_type
```

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_atom_site_U_iso_or_equiv							
_atom_site_type_symbol							
W001	1.0	0.000000	0.000000	0.496141	Uiso	1.00	W
S001	1.0	0.666667	0.333333	0.394334	Uiso	1.00	S
Se001	1.0	0.666667	0.333333	0.609525	Uiso	1.00	Se

WS₂:

```

data_created_by_vaspkit_code
_audit_creation_date      Wed Mar 11 17:32:28 2026
_pd_phase_name            'CIF files'
_cell_length_a            3.12320690
_cell_length_b            3.12320717
_cell_length_c            15.00000000
_cell_angle_alpha        90.0000
_cell_angle_beta         90.0000
_cell_angle_gamma        120.0000
_symmetry_space_group_name_H-M  'P 1'
_symmetry_Int_Tables_number  1
loop_
_symmetry_equiv_pos_as_xyz
  'x, y, z'
loop_
_atom_site_label
_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_thermal_displace_type
_atom_site_U_iso_or_equiv
_atom_site_type_symbol
W001  1.0  0.666666  0.333334  0.500000  Uiso  1.00  W
S001  1.0  0.333333  0.666667  0.395903  Uiso  1.00  S
S002  1.0  0.333333  0.666667  0.604097  Uiso  1.00  S

```