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Supporting information:

Theoretical insights into TM@PHEs as single-atom catalysts for water splitting based on density functional theory

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The structures (cif format) of single-atom catalysts:

1. Au@PHE

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_pd_phase_name                         '?
_cell_length_a                         5.70356
_cell_length_b                         5.70356
_cell_length_c                         30.35972
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_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_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   C1         1.0     0.666667      0.333333      0.515980     Biso  1.000000 C
   C2         1.0     0.327866      0.408914      0.498798     Biso  1.000000 C
   C3         1.0     0.591086      0.918951      0.498798     Biso  1.000000 C
   C4         1.0     0.081048      0.672134      0.498798     Biso  1.000000 C
   C5         1.0     0.081049      0.408913      0.498798     Biso  1.000000 C
   C6         1.0     0.591087      0.672135      0.498798     Biso  1.000000 C
   C7         1.0     0.327866      0.918950      0.498798     Biso  1.000000 C
   C8         1.0     0.384632      0.192316      0.505011     Biso  1.000000 C
   C9         1.0     0.807684      0.192315      0.505011     Biso  1.000000 C
   C10        1.0     0.807685      0.615368      0.505011     Biso  1.000000 C
   Au1        1.0     0.666667      0.333333      0.586196     Biso  1.000000 Au
```

2. Co@PHE

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_pd_phase_name                         '?
_cell_length_a                         5.78812
_cell_length_b                         5.78812
_cell_length_c                         29.47958
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_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_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   C1         1.0     0.666764     0.333236     0.502281     Biso  1.000000 C
   C2         1.0     0.327373     0.408581     0.501373     Biso  1.000000 C
   C3         1.0     0.591456     0.918528     0.501369     Biso  1.000000 C
   C4         1.0     0.081465     0.672644     0.501370     Biso  1.000000 C
   C5         1.0     0.081472     0.408543     0.501369     Biso  1.000000 C
   C6         1.0     0.591420     0.672629     0.501373     Biso  1.000000 C
   C7         1.0     0.327355     0.918534     0.501370     Biso  1.000000 C
   C8         1.0     0.390147     0.194947     0.502194     Biso  1.000000 C
   C9         1.0     0.805081     0.194918     0.502190     Biso  1.000000 C
   C10        1.0     0.805053     0.609854     0.502194     Biso  1.000000 C
   Co1        1.0     0.333420     0.666580     0.552917     Biso  1.000000 Co
```

3. Cu@PHE

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_pd_phase_name                         '?
_cell_length_a                         5.64145
_cell_length_b                         5.64145
_cell_length_c                         31.03191
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_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_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   C1         1.0     0.666667     0.333333     0.520035     Biso  1.000000 C
   C2         1.0     0.331586     0.413391     0.495652     Biso  1.000000 C
   C3         1.0     0.586608     0.918194     0.495652     Biso  1.000000 C
   C4         1.0     0.081806     0.668414     0.495652     Biso  1.000000 C
   C5         1.0     0.081806     0.413391     0.495652     Biso  1.000000 C
   C6         1.0     0.586610     0.668415     0.495652     Biso  1.000000 C
   C7         1.0     0.331585     0.918193     0.495652     Biso  1.000000 C
   C8         1.0     0.380948     0.190473     0.510019     Biso  1.000000 C
   C9         1.0     0.809526     0.190473     0.510019     Biso  1.000000 C
   C10        1.0     0.809527     0.619053     0.510019     Biso  1.000000 C
   Cu1        1.0     0.000000     0.000000     0.545996     Biso  1.000000 Cu
```

4. Fe@PHE

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_pd_phase_name                         '?
_cell_length_a                         5.65186
_cell_length_b                         5.65186
_cell_length_c                         30.91773
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_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_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   C1         1.0     0.666667     0.333333     0.520380     Biso  1.000000 C
   C2         1.0     0.331266     0.413274     0.495610     Biso  1.000000 C
   C3         1.0     0.586726     0.917991     0.495610     Biso  1.000000 C
   C4         1.0     0.082008     0.668734     0.495610     Biso  1.000000 C
   C5         1.0     0.082009     0.413273     0.495610     Biso  1.000000 C
   C6         1.0     0.586727     0.668735     0.495610     Biso  1.000000 C
   C7         1.0     0.331266     0.917990     0.495610     Biso  1.000000 C
   C8         1.0     0.381009     0.190504     0.510401     Biso  1.000000 C
   C9         1.0     0.809496     0.190503     0.510401     Biso  1.000000 C
   C10        1.0     0.809496     0.618992     0.510401     Biso  1.000000 C
   Fe1        1.0     0.000000     0.000000     0.544760     Biso  1.000000 Fe
```

5. Ni@PHE

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_pd_phase_name                         '?
_cell_length_a                         5.58347
_cell_length_b                         5.58347
_cell_length_c                         31.67977
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_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_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   C1         1.0     0.666667     0.333333     0.522930     Biso  1.000000 C
   C2         1.0     0.331962     0.412550     0.494786     Biso  1.000000 C
   C3         1.0     0.587450     0.919411     0.494786     Biso  1.000000 C
   C4         1.0     0.080589     0.668038     0.494786     Biso  1.000000 C
   C5         1.0     0.080589     0.412549     0.494786     Biso  1.000000 C
   C6         1.0     0.587451     0.668039     0.494786     Biso  1.000000 C
   C7         1.0     0.331961     0.919410     0.494786     Biso  1.000000 C
   C8         1.0     0.375588     0.187794     0.511355     Biso  1.000000 C
   C9         1.0     0.812206     0.187793     0.511355     Biso  1.000000 C
   C10        1.0     0.812207     0.624412     0.511355     Biso  1.000000 C
   Ni1        1.0     0.000000     0.000000     0.544289     Biso  1.000000 Ni
```

6. Pd@PHE

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_pd_phase_name                         '?
_cell_length_a                         5.59074
_cell_length_b                         5.59074
_cell_length_c                         31.59735
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_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_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   C1         1.0     0.666667     0.333333     0.522224     Biso  1.000000 C
   C2         1.0     0.332331     0.413069     0.494041     Biso  1.000000 C
   C3         1.0     0.586931     0.919260     0.494041     Biso  1.000000 C
   C4         1.0     0.080739     0.667670     0.494041     Biso  1.000000 C
   C5         1.0     0.080740     0.413068     0.494041     Biso  1.000000 C
   C6         1.0     0.586932     0.667671     0.494041     Biso  1.000000 C
   C7         1.0     0.332330     0.919259     0.494041     Biso  1.000000 C
   C8         1.0     0.377326     0.188662     0.510571     Biso  1.000000 C
   C9         1.0     0.811337     0.188662     0.510571     Biso  1.000000 C
   C10        1.0     0.811338     0.622674     0.510571     Biso  1.000000 C
   Pd1        1.0     0.000000     0.000000     0.551819     Biso  1.000000 Pd
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7. Pt@PHE

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_pd_phase_name                         '?
_cell_length_a                         5.55388
_cell_length_b                         5.55388
_cell_length_c                         32.01822
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_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_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   C1         1.0     0.666667     0.333333     0.523773     Biso  1.000000 C
   C2         1.0     0.332568     0.412619     0.493361     Biso  1.000000 C
   C3         1.0     0.587381     0.919948     0.493361     Biso  1.000000 C
   C4         1.0     0.080051     0.667432     0.493361     Biso  1.000000 C
   C5         1.0     0.080052     0.412618     0.493361     Biso  1.000000 C
   C6         1.0     0.587382     0.667433     0.493361     Biso  1.000000 C
   C7         1.0     0.332567     0.919947     0.493361     Biso  1.000000 C
   C8         1.0     0.372892     0.186445     0.511565     Biso  1.000000 C
   C9         1.0     0.813554     0.186445     0.511565     Biso  1.000000 C
   C10        1.0     0.813555     0.627109     0.511565     Biso  1.000000 C
   Pt1        1.0     0.000000     0.000000     0.551365     Biso  1.000000 Pt
```

8. Ru@PHE

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_pd_phase_name                         '?
_cell_length_a                         5.78788
_cell_length_b                         5.78788
_cell_length_c                         29.48211
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_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_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   C1         1.0     0.666764     0.333236     0.503415     Biso  1.000000 C
   C2         1.0     0.328045     0.409021     0.500464     Biso  1.000000 C
   C3         1.0     0.591017     0.918760     0.500459     Biso  1.000000 C
   C4         1.0     0.081232     0.671972     0.500460     Biso  1.000000 C
   C5         1.0     0.081240     0.408983     0.500459     Biso  1.000000 C
   C6         1.0     0.590980     0.671957     0.500464     Biso  1.000000 C
   C7         1.0     0.328027     0.918767     0.500460     Biso  1.000000 C
   C8         1.0     0.389879     0.194813     0.502479     Biso  1.000000 C
   C9         1.0     0.805215     0.194785     0.502476     Biso  1.000000 C
   C10        1.0     0.805187     0.610121     0.502479     Biso  1.000000 C
   Ru1        1.0     0.333420     0.666580     0.556385     Biso  1.000000 Ru
```

9. Sc@PHE

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_pd_phase_name                         '?
_cell_length_a                         5.67311
_cell_length_b                         5.67311
_cell_length_c                         30.68644
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_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_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   C1         1.0     0.666667     0.333333     0.487873     Biso  1.000000 C
   C2         1.0     0.330763     0.409665     0.510983     Biso  1.000000 C
   C3         1.0     0.590335     0.921097     0.510983     Biso  1.000000 C
   C4         1.0     0.078903     0.669238     0.510983     Biso  1.000000 C
   C5         1.0     0.078903     0.409664     0.510983     Biso  1.000000 C
   C6         1.0     0.590336     0.669239     0.510983     Biso  1.000000 C
   C7         1.0     0.330762     0.921096     0.510983     Biso  1.000000 C
   C8         1.0     0.386766     0.193382     0.499326     Biso  1.000000 C
   C9         1.0     0.806617     0.193382     0.499326     Biso  1.000000 C
   C10        1.0     0.806618     0.613235     0.499326     Biso  1.000000 C
   Sc1        1.0     0.666667     0.333333     0.558250     Biso  1.000000 Sc
```

10. Ti@PHE

```
#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_pd_phase_name                         '?
_cell_length_a                         5.66409
_cell_length_b                         5.66409
_cell_length_c                         30.78429
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_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_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   C1         1.0     0.666667     0.333333     0.486565     Biso  1.000000 C
   C2         1.0     0.330648     0.409045     0.511825     Biso  1.000000 C
   C3         1.0     0.590955     0.921603     0.511825     Biso  1.000000 C
   C4         1.0     0.078397     0.669352     0.511825     Biso  1.000000 C
   C5         1.0     0.078397     0.409044     0.511825     Biso  1.000000 C
   C6         1.0     0.590956     0.669353     0.511825     Biso  1.000000 C
   C7         1.0     0.330648     0.921602     0.511825     Biso  1.000000 C
   C8         1.0     0.387209     0.193604     0.499227     Biso  1.000000 C
   C9         1.0     0.806396     0.193604     0.499227     Biso  1.000000 C
   C10        1.0     0.806396     0.612791     0.499227     Biso  1.000000 C
   Ti1        1.0     0.666667     0.333333     0.554802     Biso  1.000000 Ti
```

11. V@PHE

```
#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_pd_phase_name                         '□□2_layer1                              '
_cell_length_a                         5.69679
_cell_length_b                         5.69679
_cell_length_c                         30.43194
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_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_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   C1         1.0     0.666667      0.333333      0.488238     Biso  1.000000 C
   C2         1.0     0.329430      0.410434      0.510708     Biso  1.000000 C
   C3         1.0     0.589566      0.918994      0.510708     Biso  1.000000 C
   C4         1.0     0.081005      0.670571      0.510708     Biso  1.000000 C
   C5         1.0     0.081006      0.410433      0.510708     Biso  1.000000 C
   C6         1.0     0.589567      0.670572      0.510708     Biso  1.000000 C
   C7         1.0     0.329429      0.918994      0.510708     Biso  1.000000 C
   C8         1.0     0.388588      0.194293      0.500551     Biso  1.000000 C
   C9         1.0     0.805706      0.194293      0.500551     Biso  1.000000 C
   C10        1.0     0.805707      0.611413      0.500551     Biso  1.000000 C
   V1         1.0     0.666667      0.333333      0.555860     Biso  1.000000 V
```