

Two-dimensional molybdenum carbides: potential thermoelectric materials in MXenes

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Units

Density of states (states/eV/Cell)

Carrier density ($1/\text{cm}^3$)

S ($\mu\text{V/K}$)

σ/τ [$1/(\Omega \text{ m s})$]

$S^2\sigma/\tau$ [$10^{14} \mu\text{W}/(\text{cm K}^2 \text{ s})$]

Test calculations

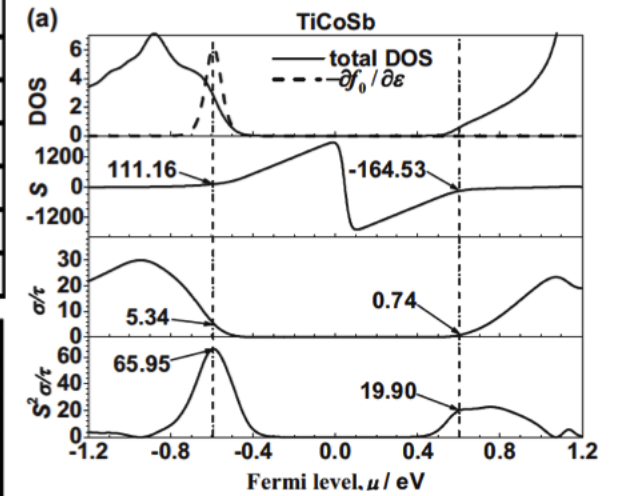
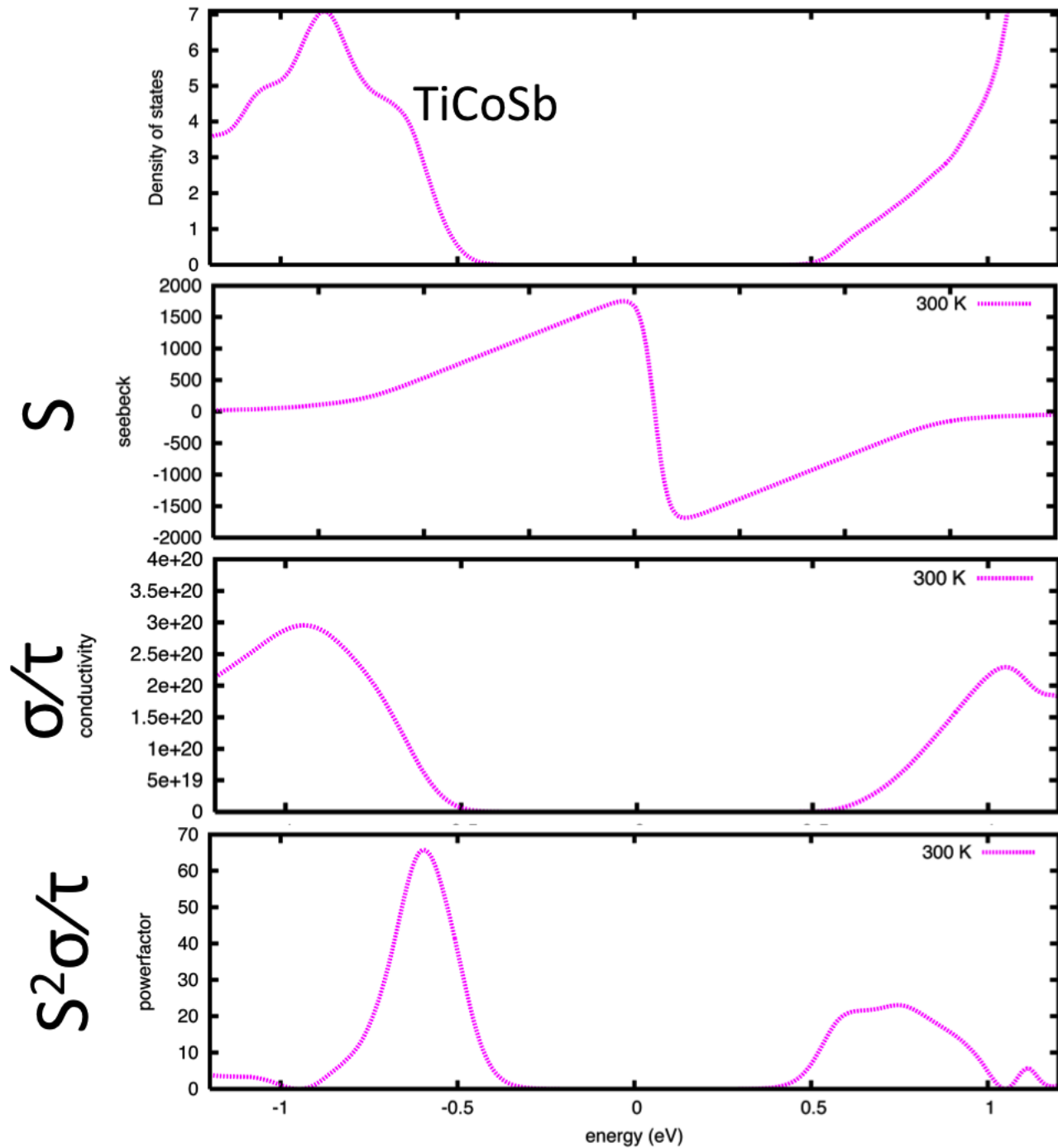


Figure 2. Density of states and electrical transport properties versus the Fermi levels for a) TiCoSb, b) ZrNiSn, and c) LaPdBi. The units for DOS, σ/τ , S , and $S^2\sigma/\tau$ are $\text{state eV}^{-1} \text{ u.c.}^{-1}$, $10^{17} \Omega^{-1} \text{ cm}^{-1} \text{ s}^{-1}$, $\mu\text{V K}^{-1}$, and $10^{14} \mu\text{W cm}^{-1} \text{ K}^{-2} \text{ s}^{-1}$, respectively. We label the maximum power factor for each compound and the corresponding S and σ/τ . In the DOS panel of each HH system, the energy dependence of $-\partial f_0 / \partial \epsilon$ is illustrated.

Ref. Adv. Fun. Mater 18, 2880 (2008)

TEST calculation

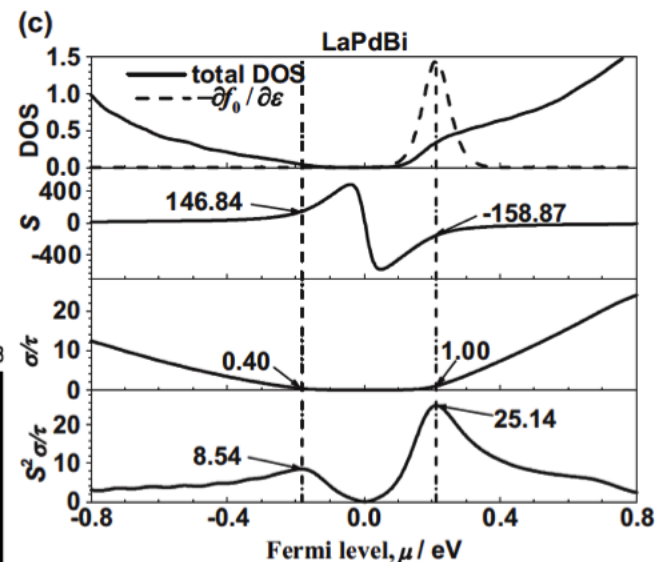
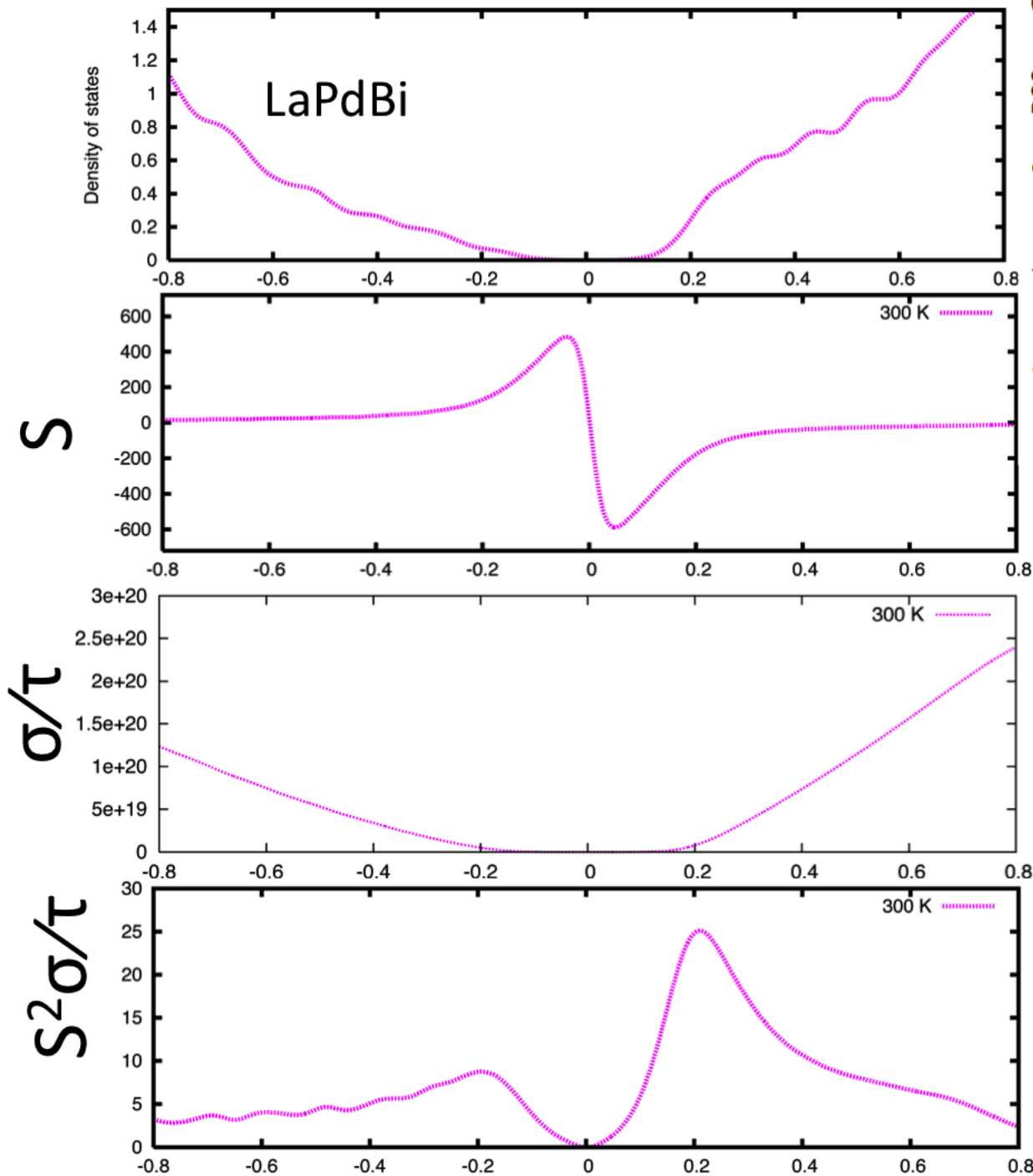


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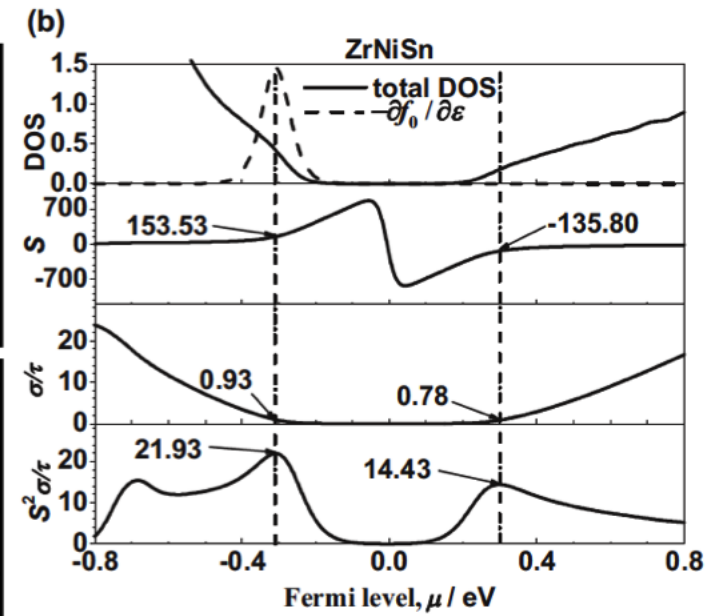
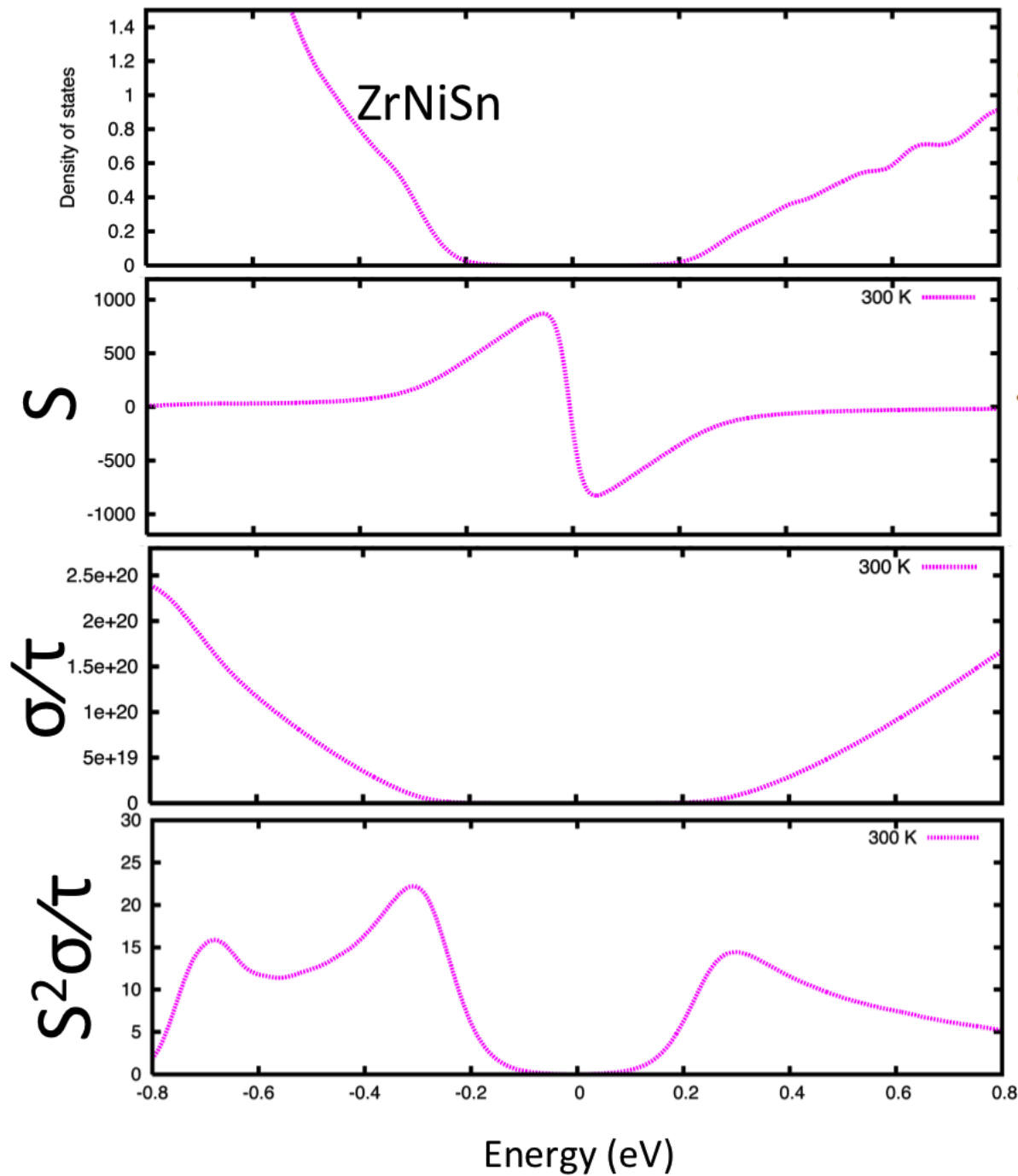


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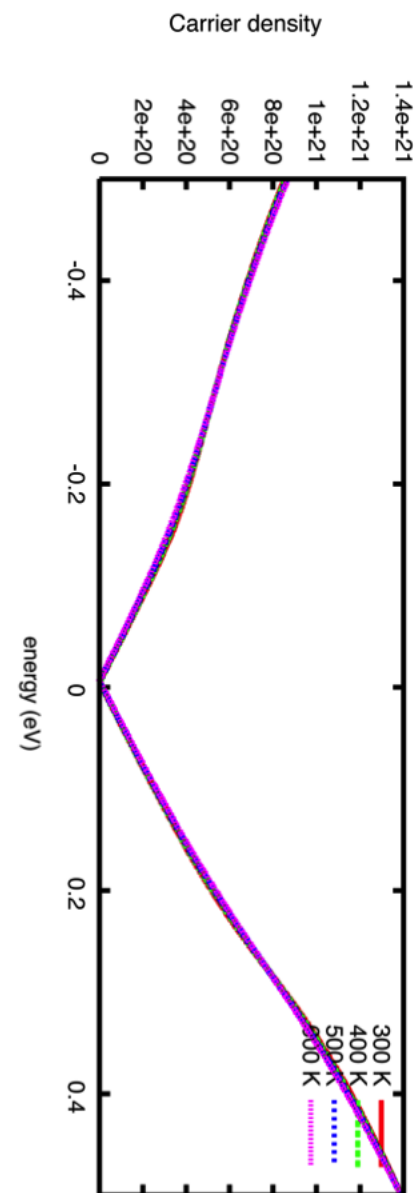
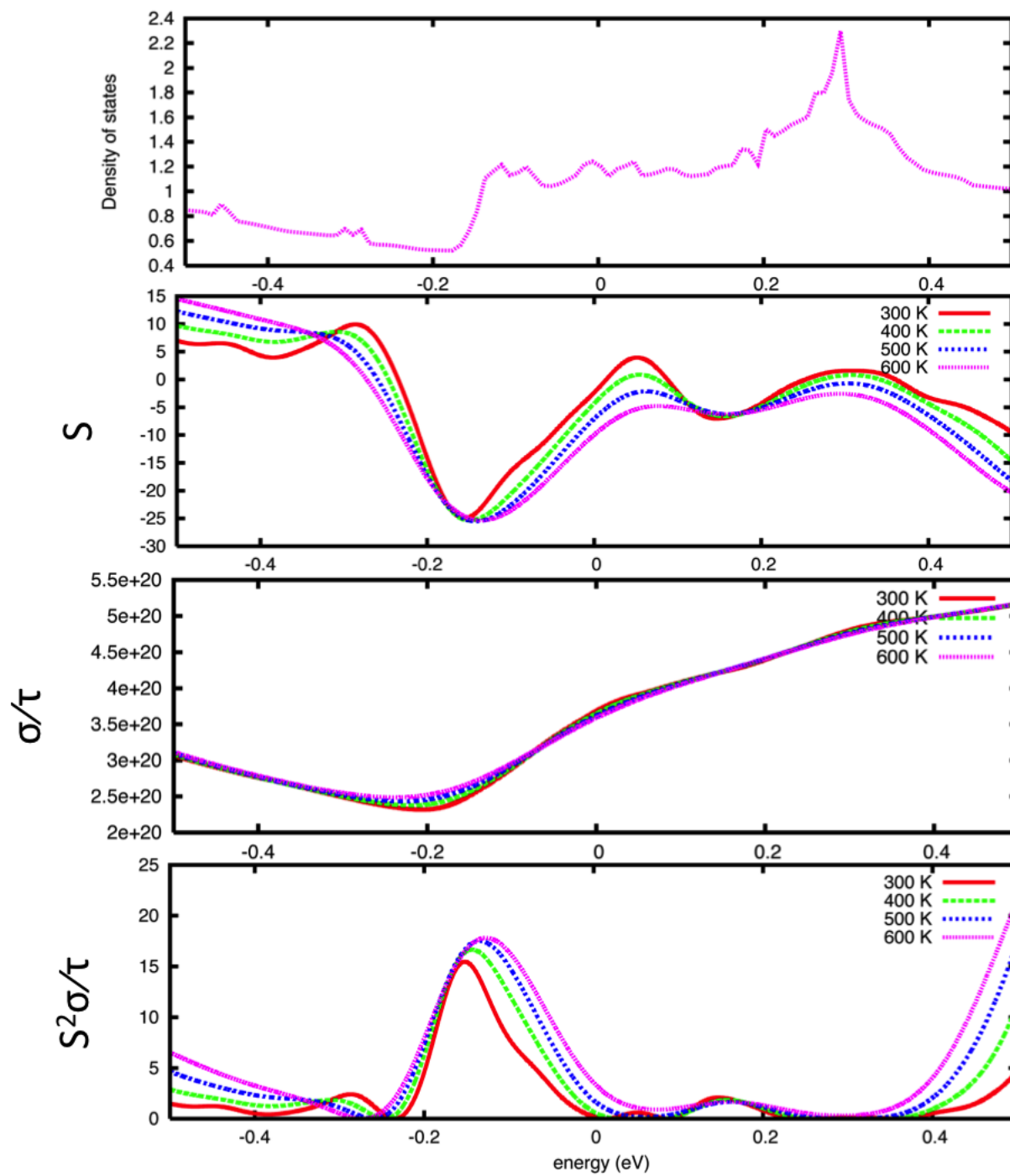
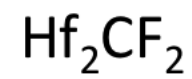
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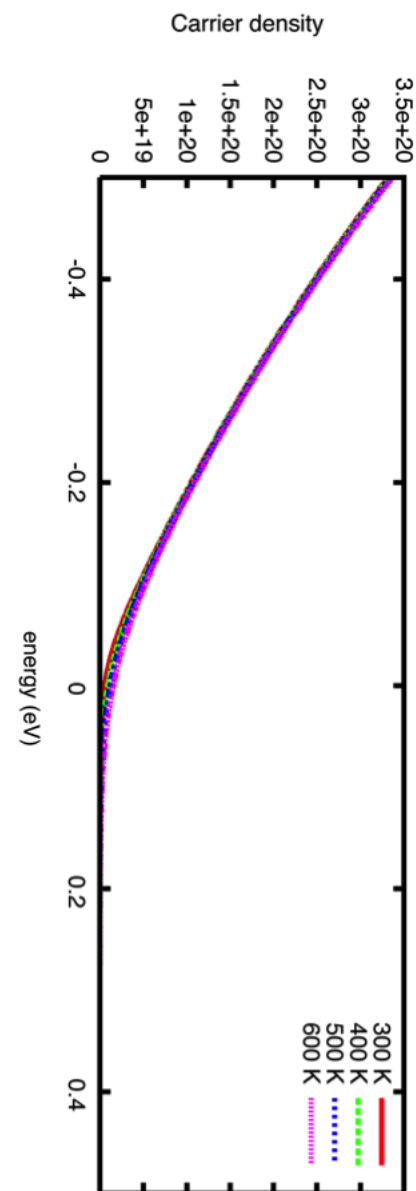
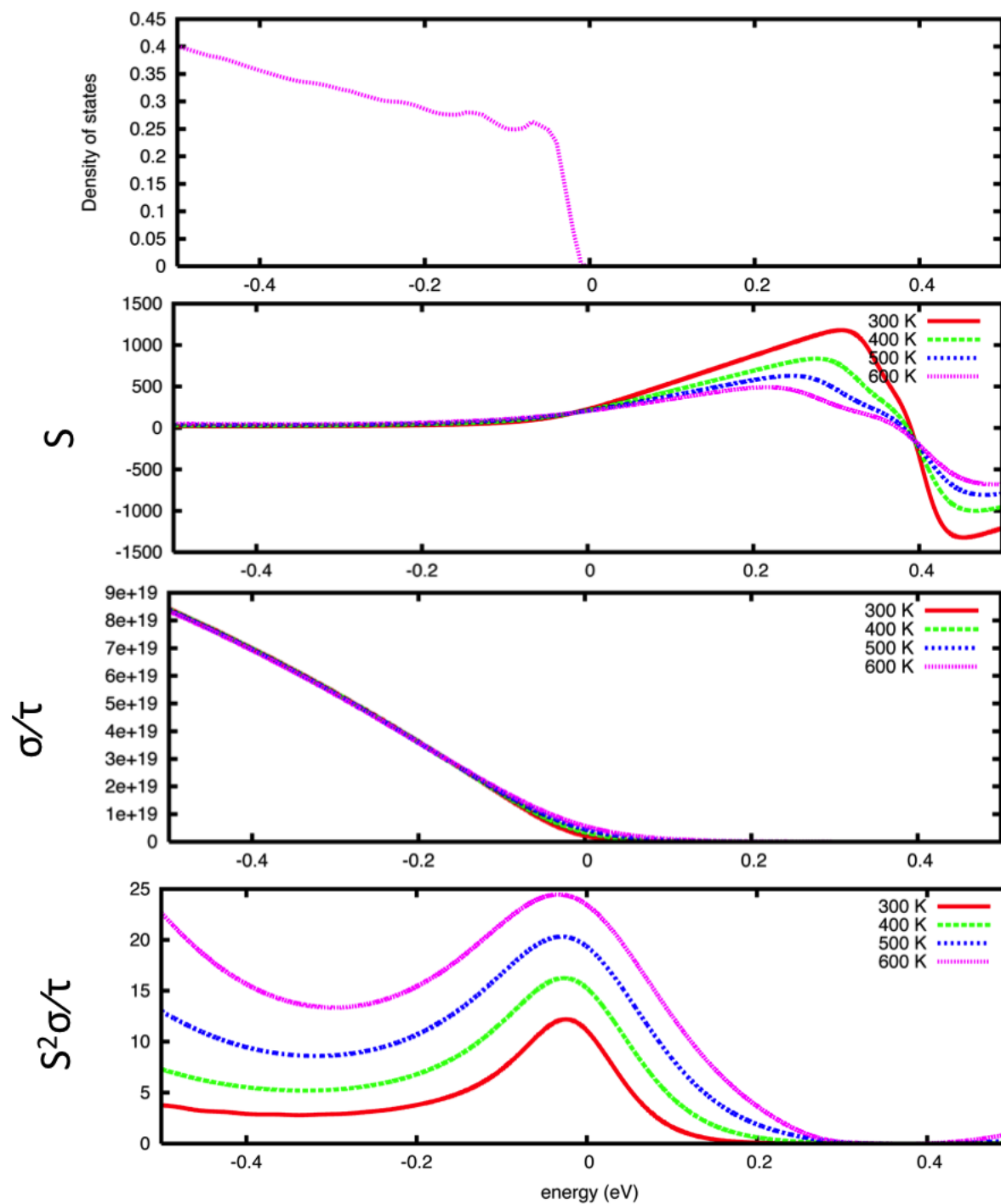
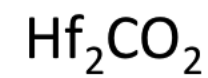
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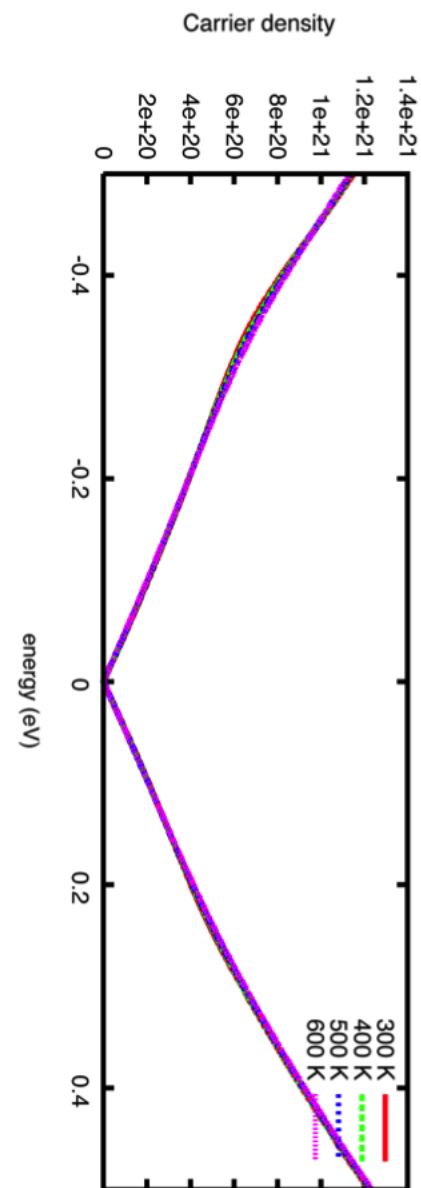
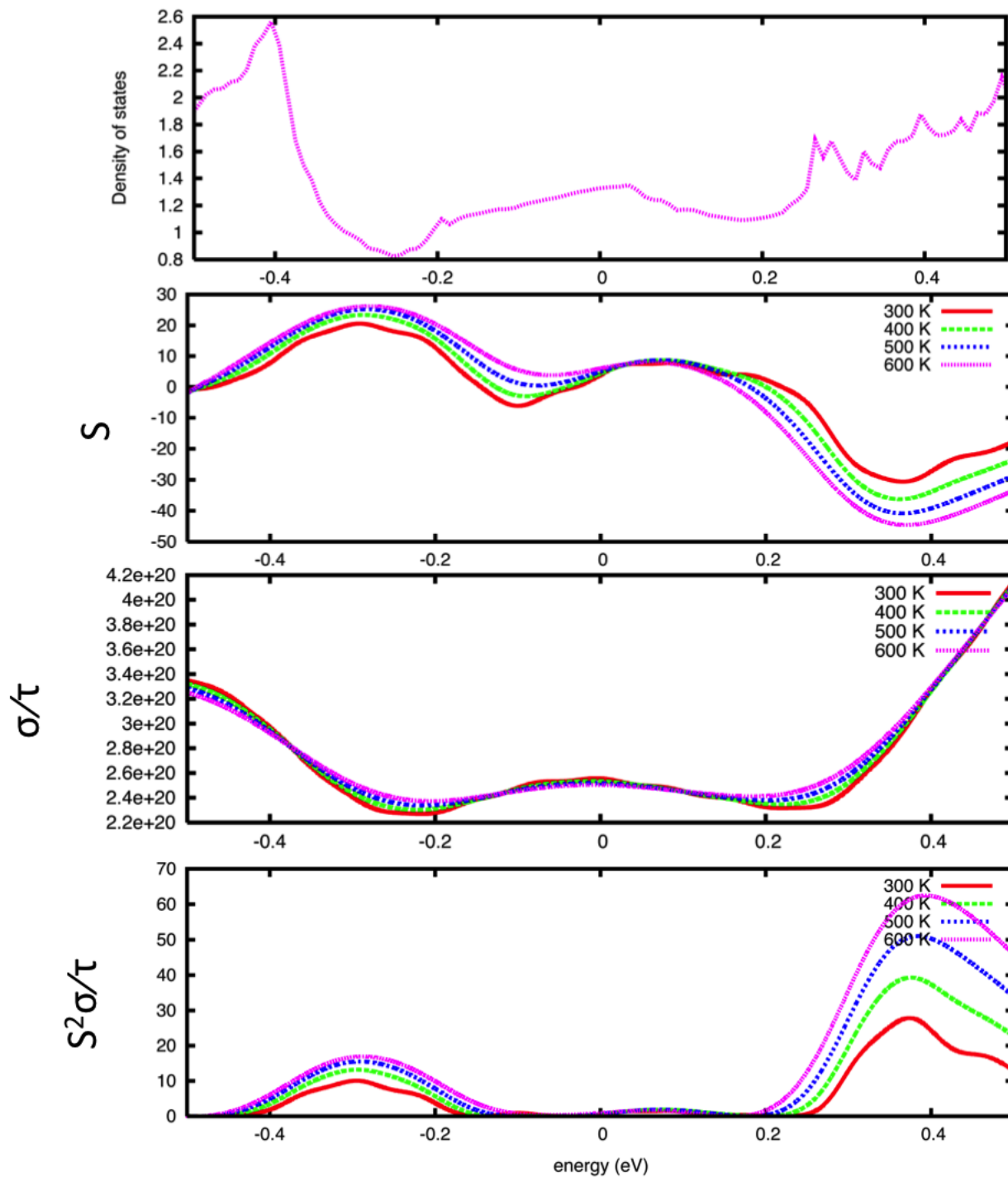
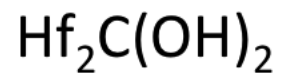
Thermoelectric properties of multilayer MXenes

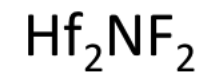
$$S = (S_{xx} + S_{yy} + S_{zz})/3$$

$$\sigma = (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3$$

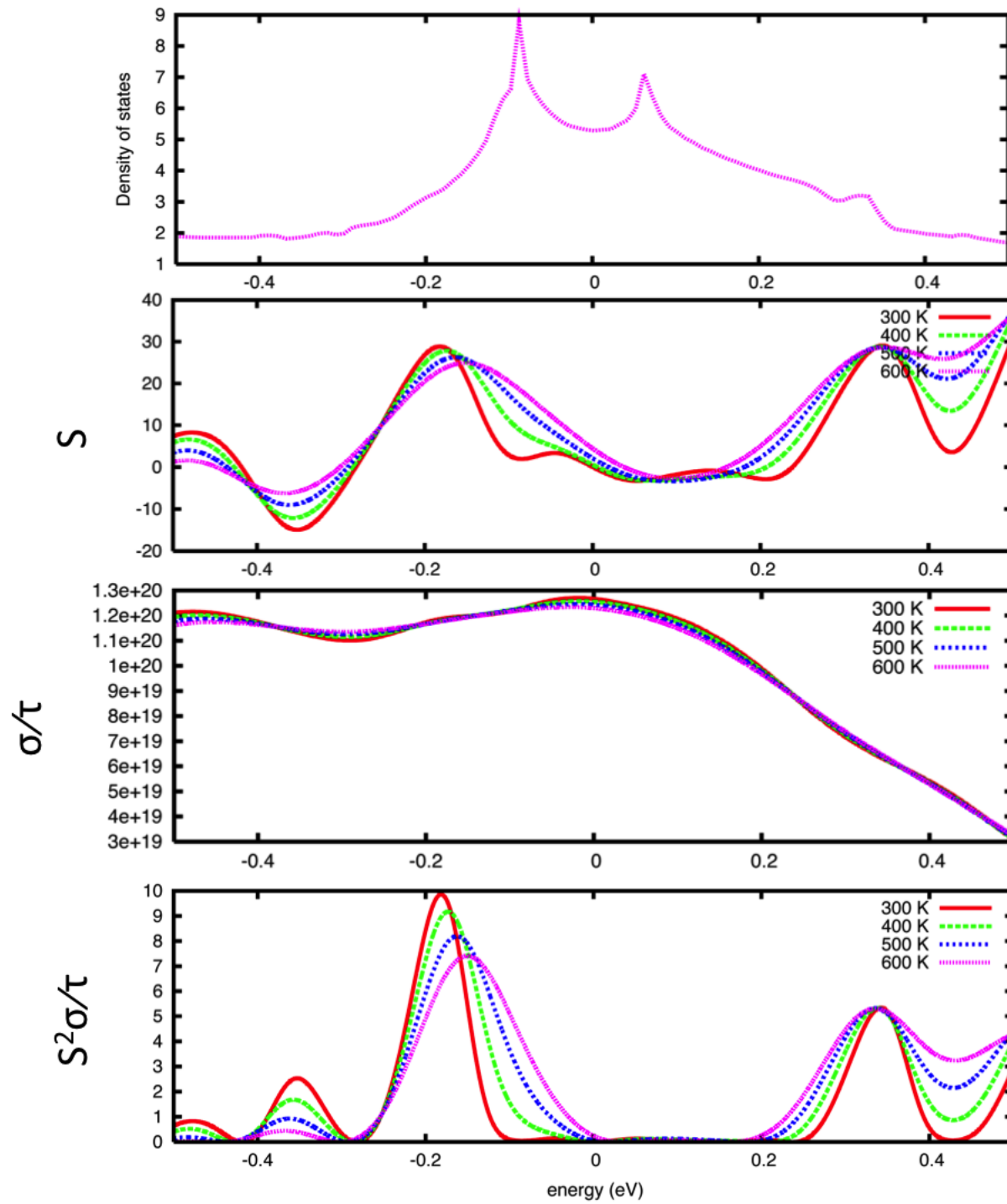
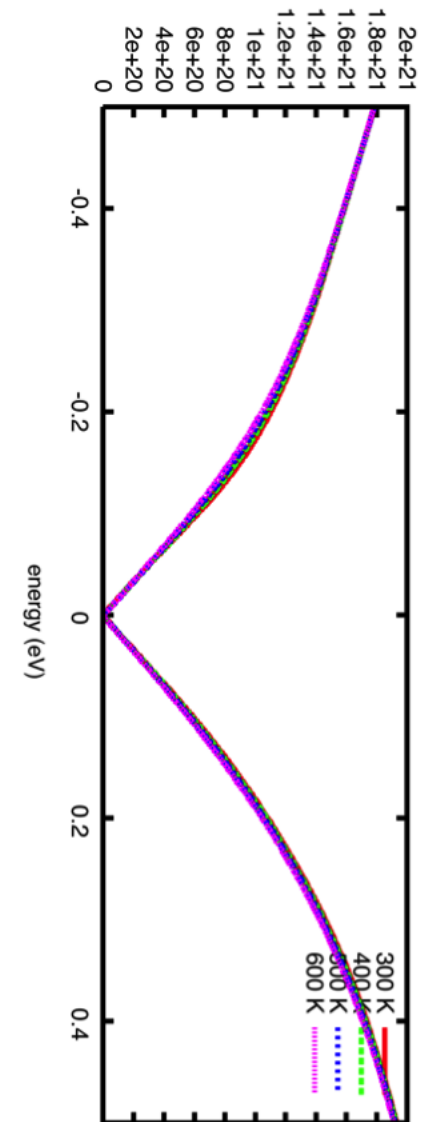


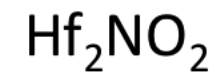




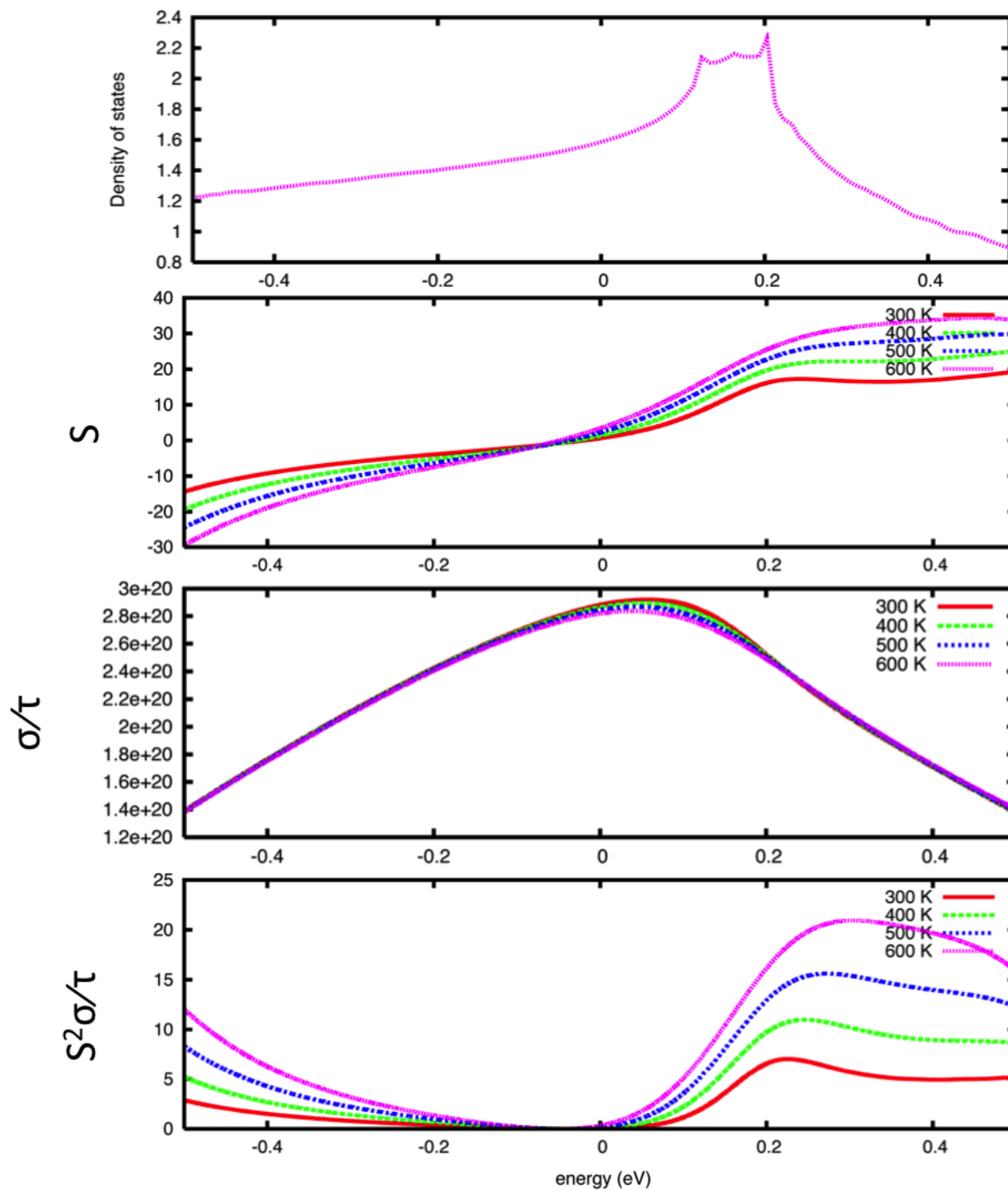
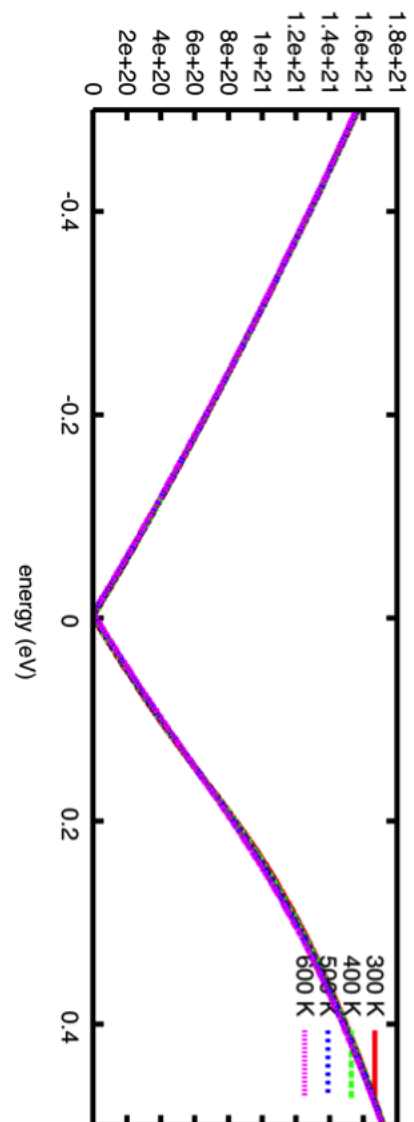


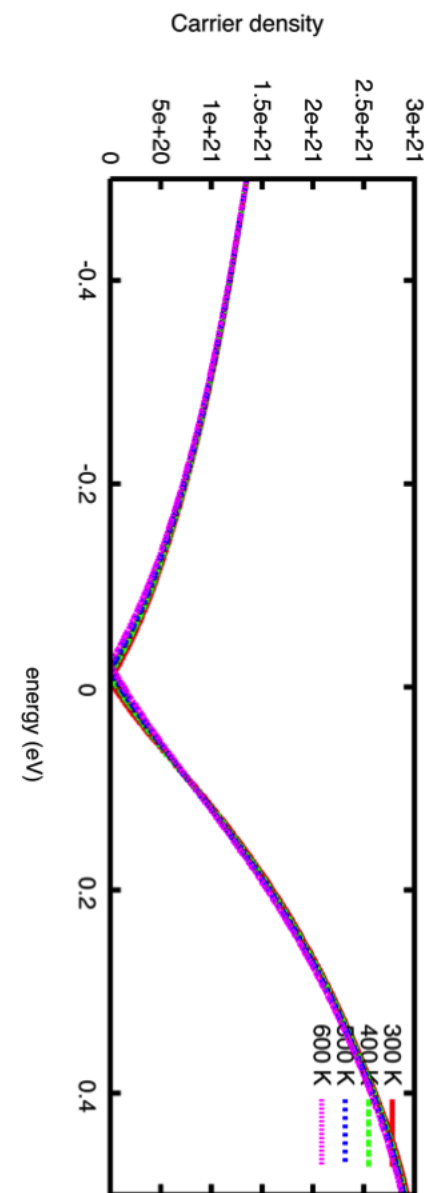
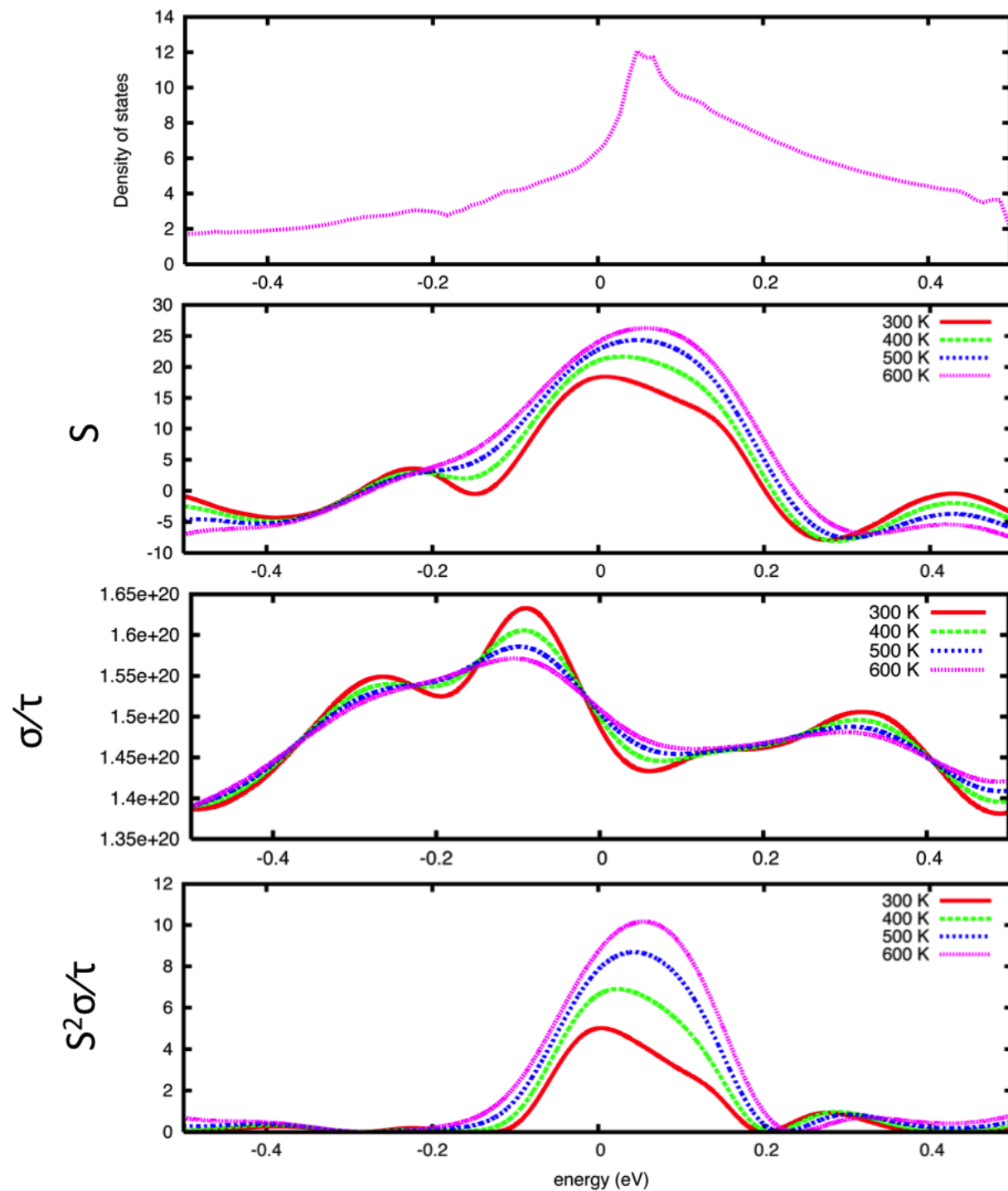
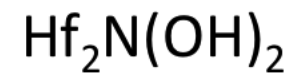
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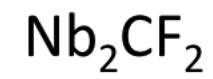




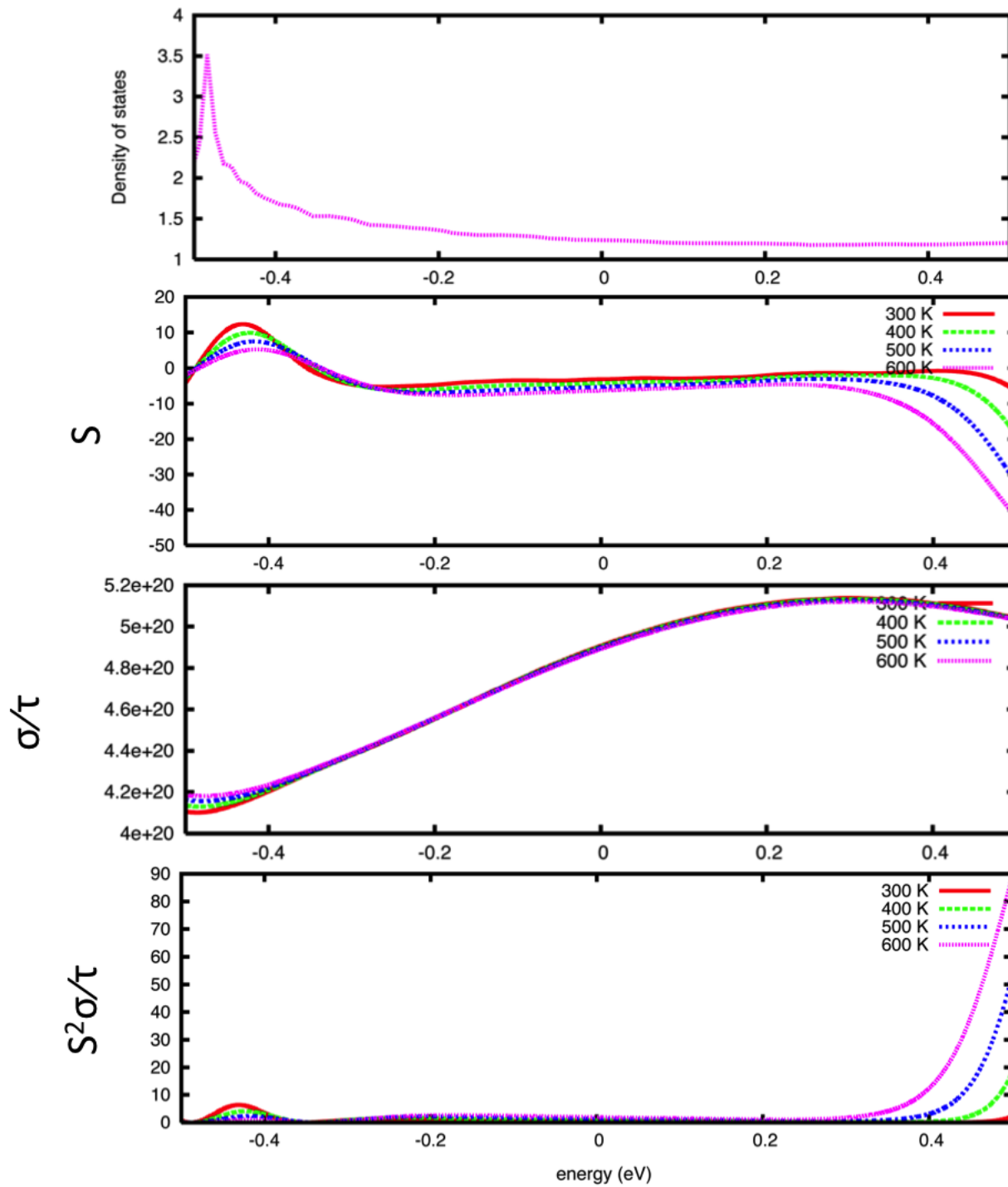
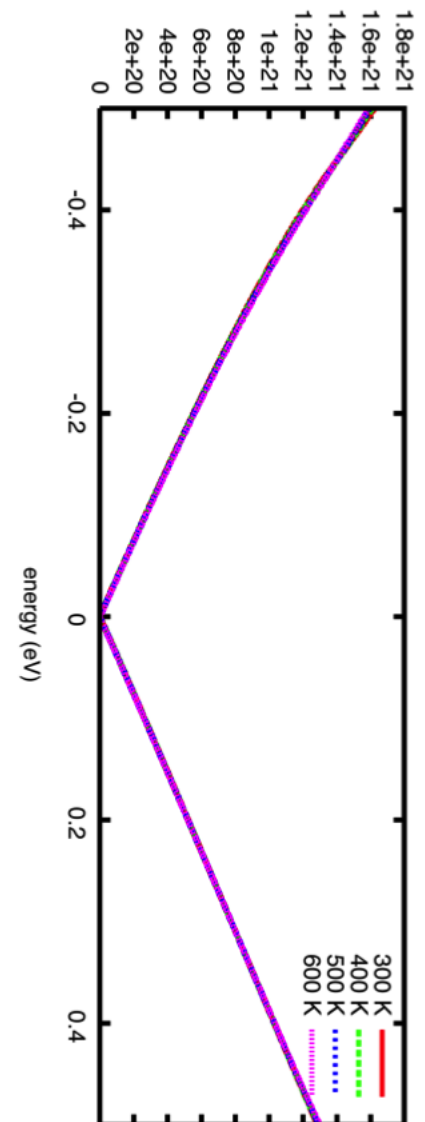
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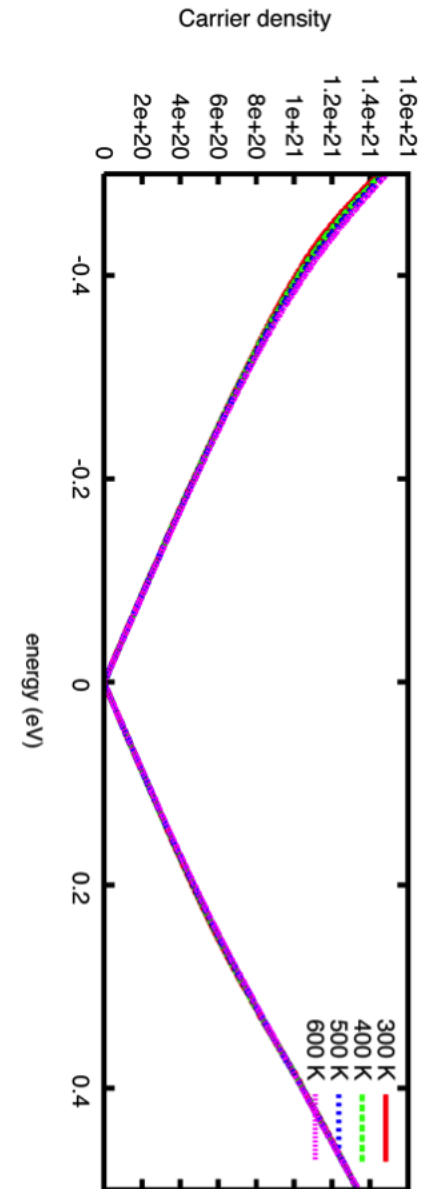
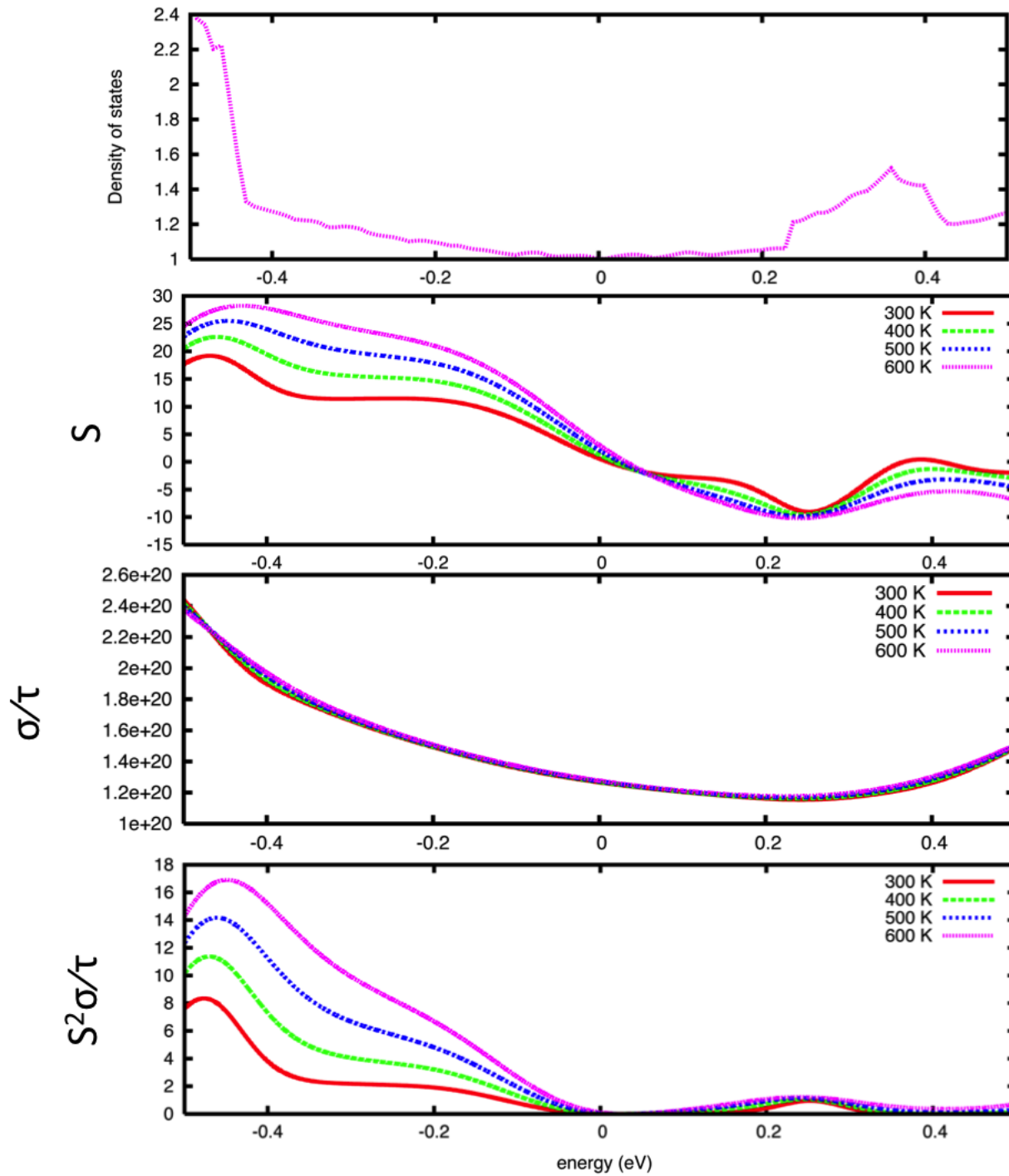
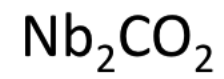


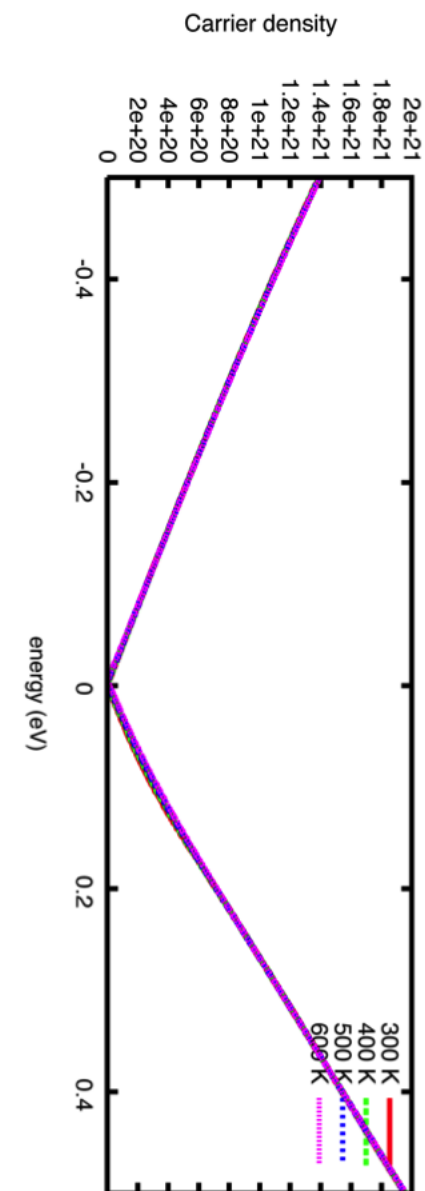
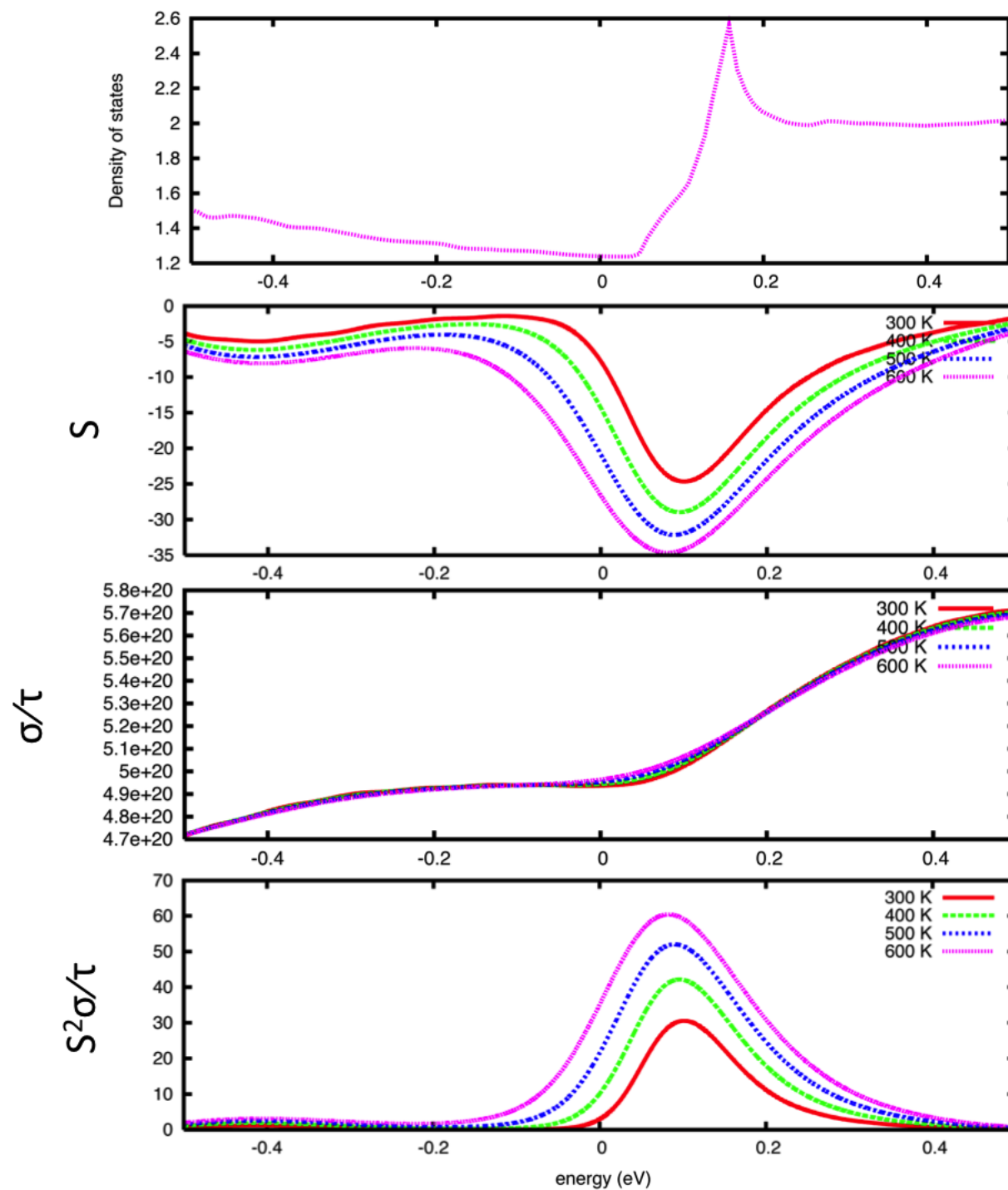
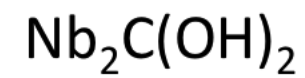


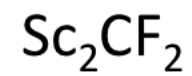


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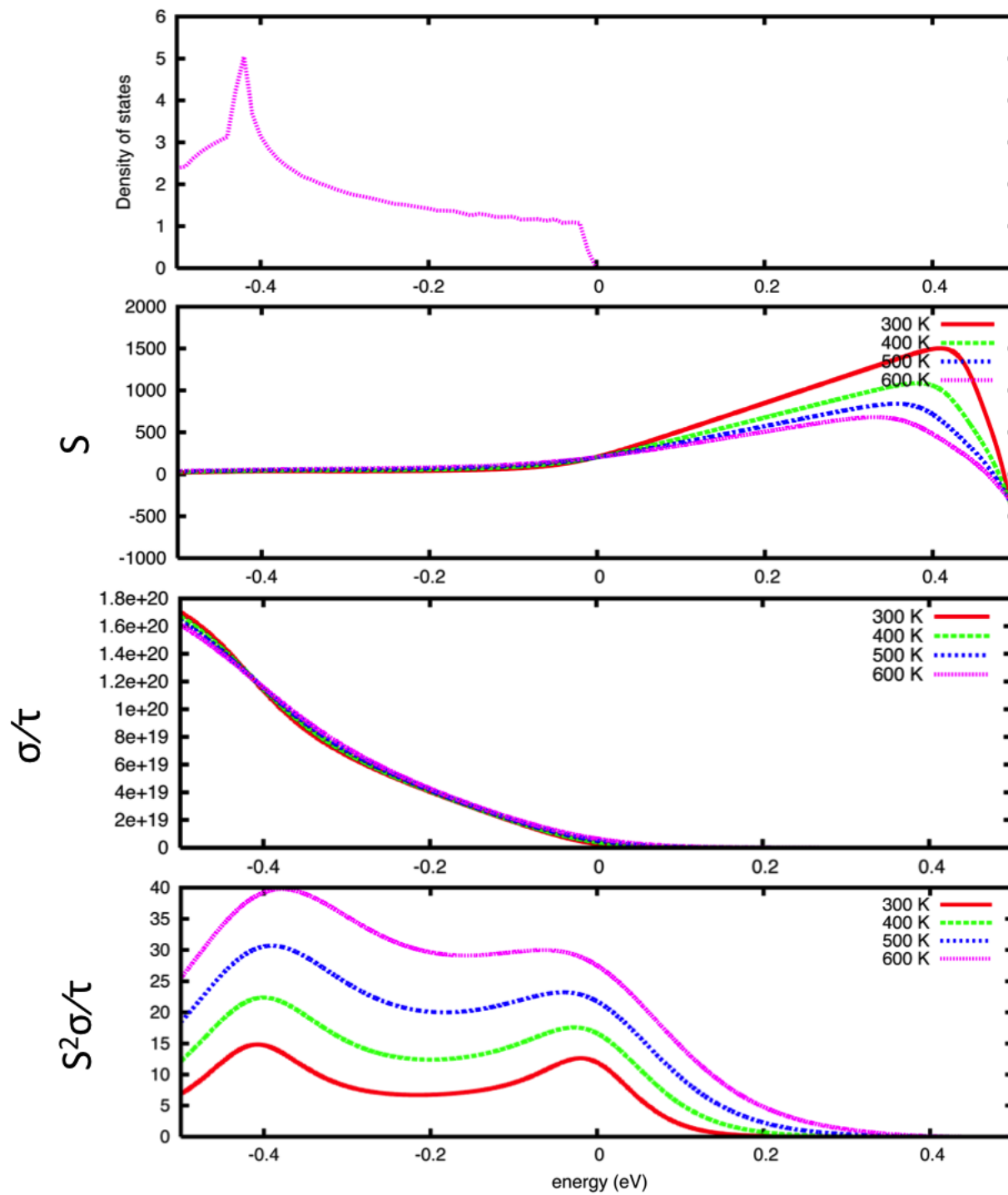
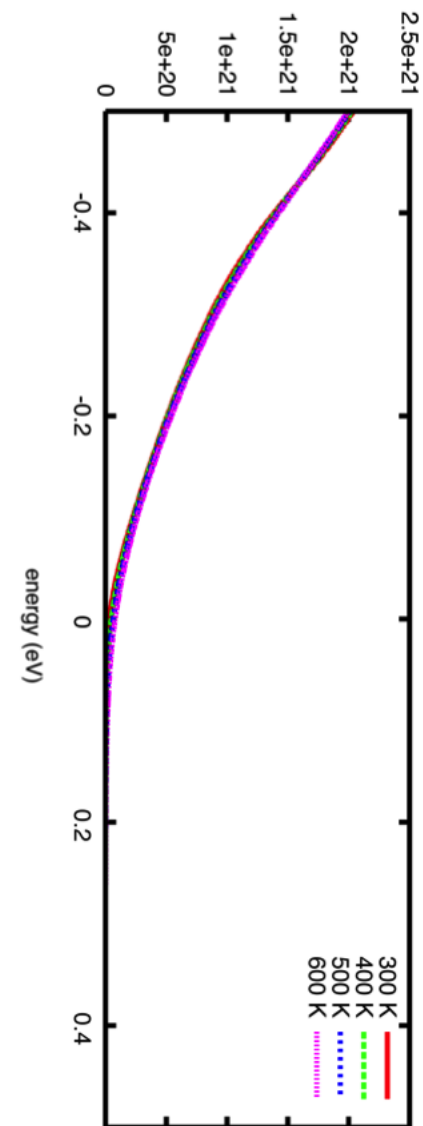


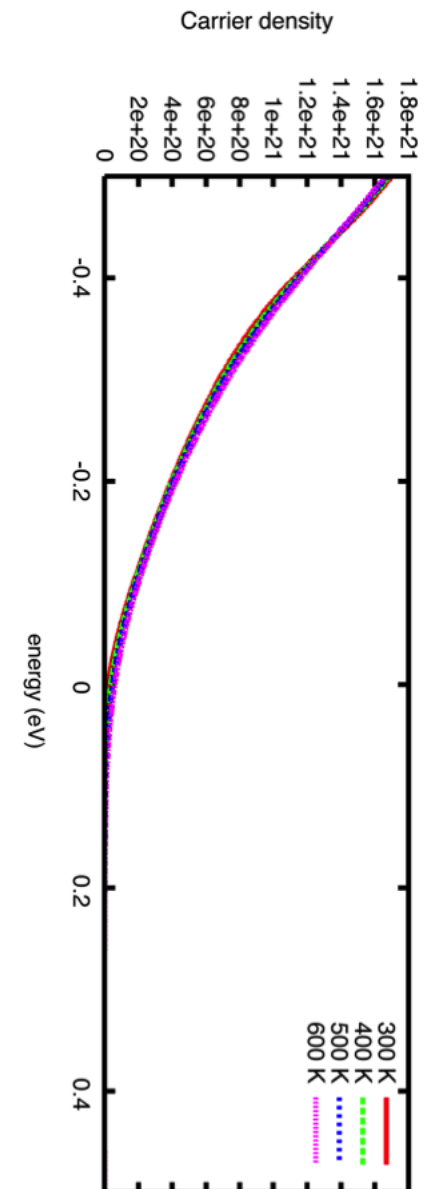
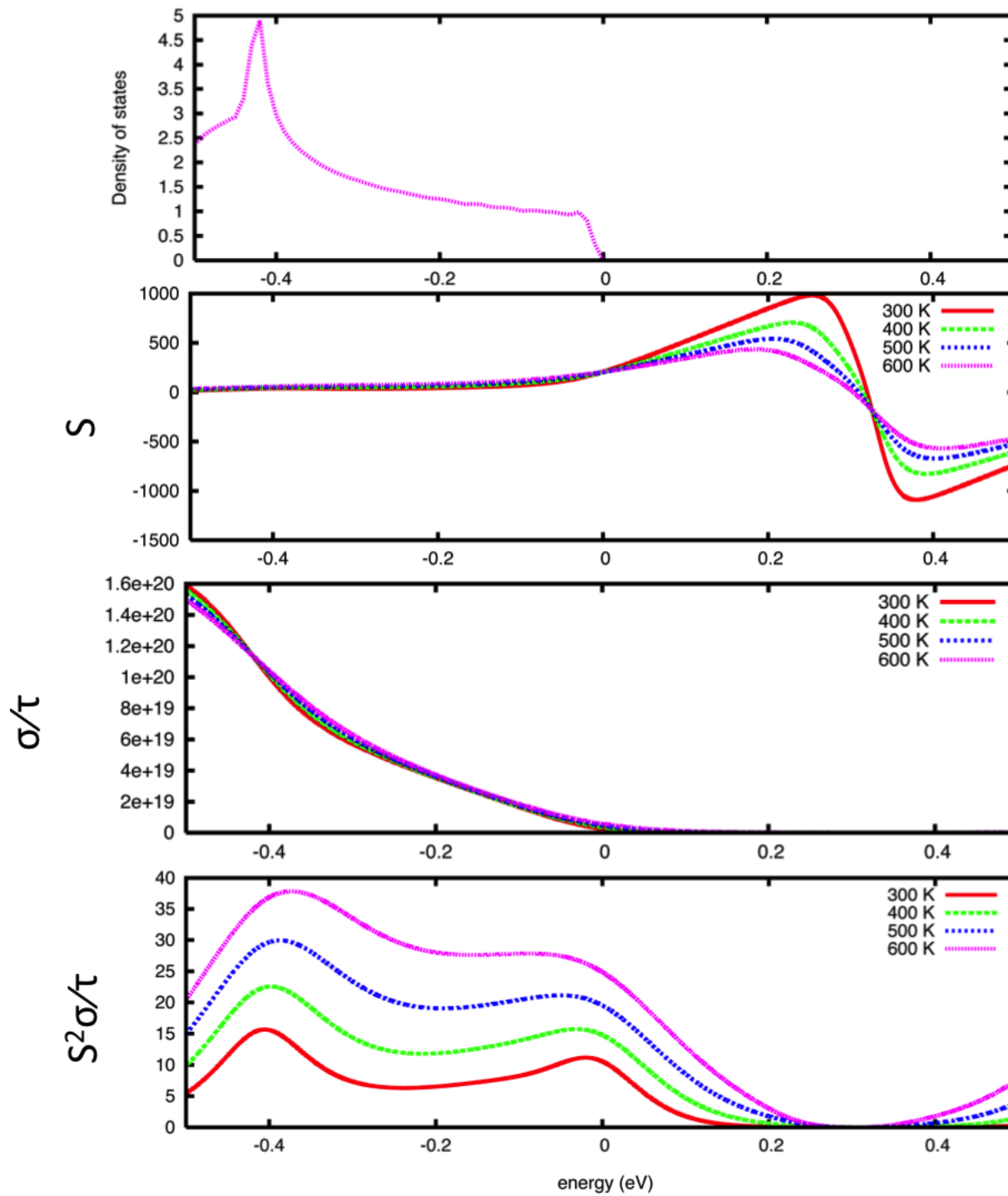
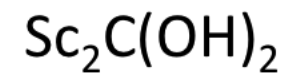


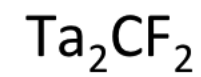




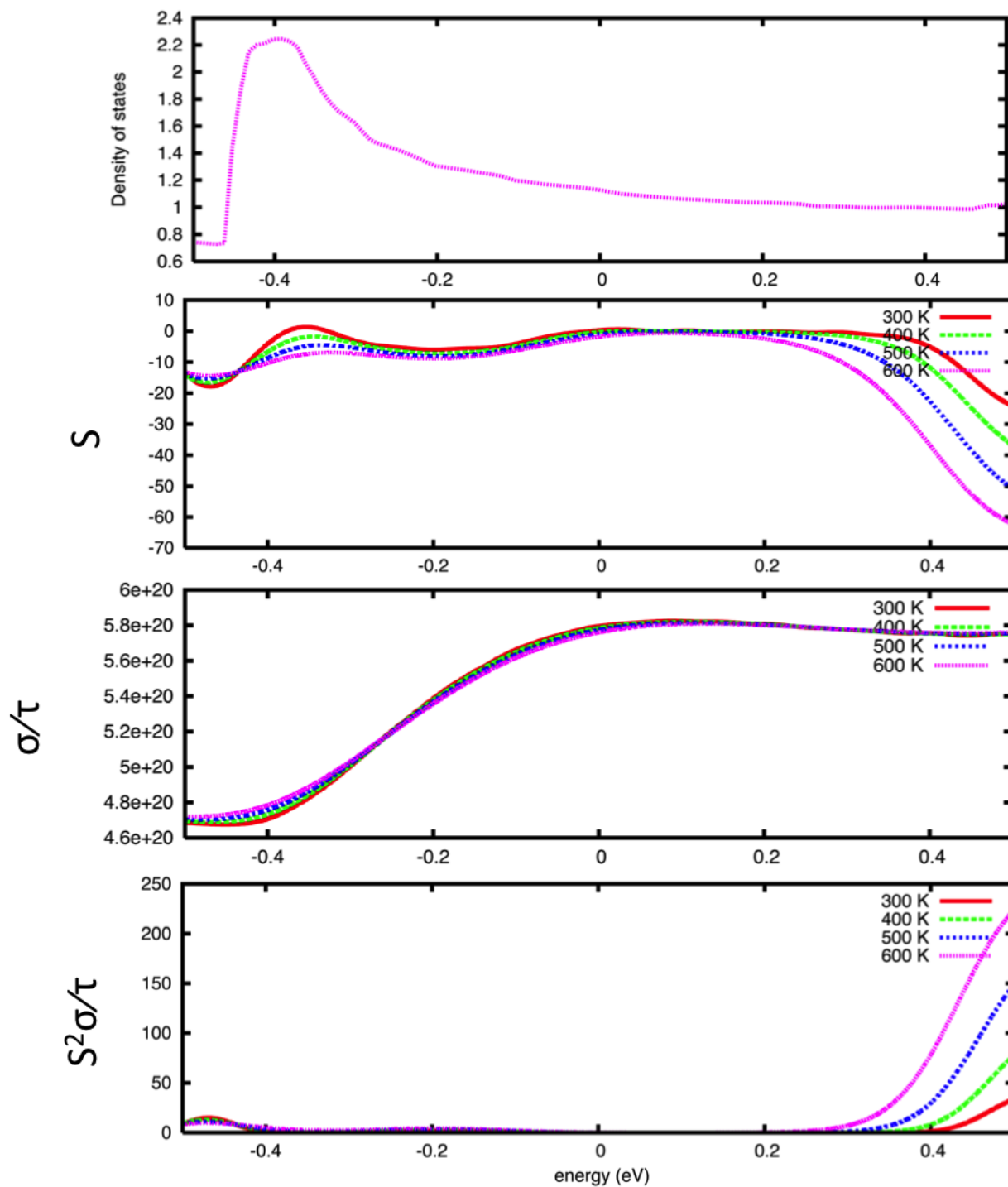
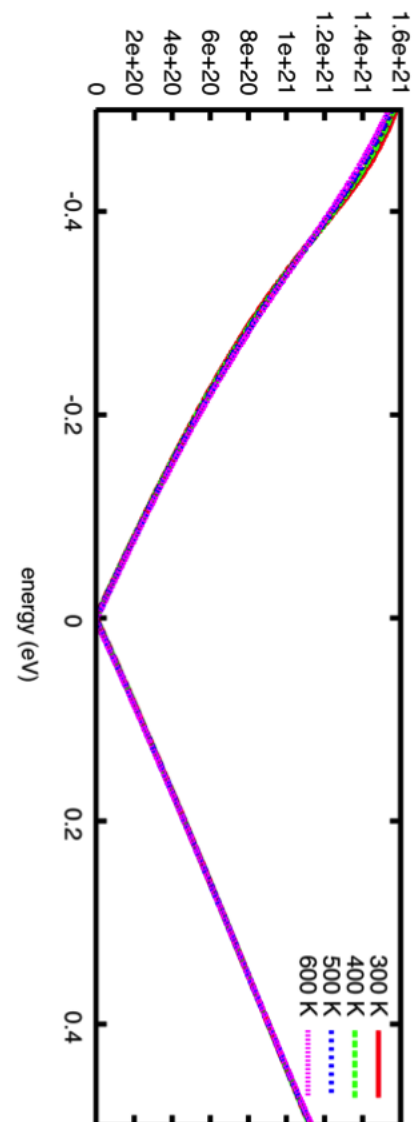
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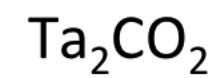




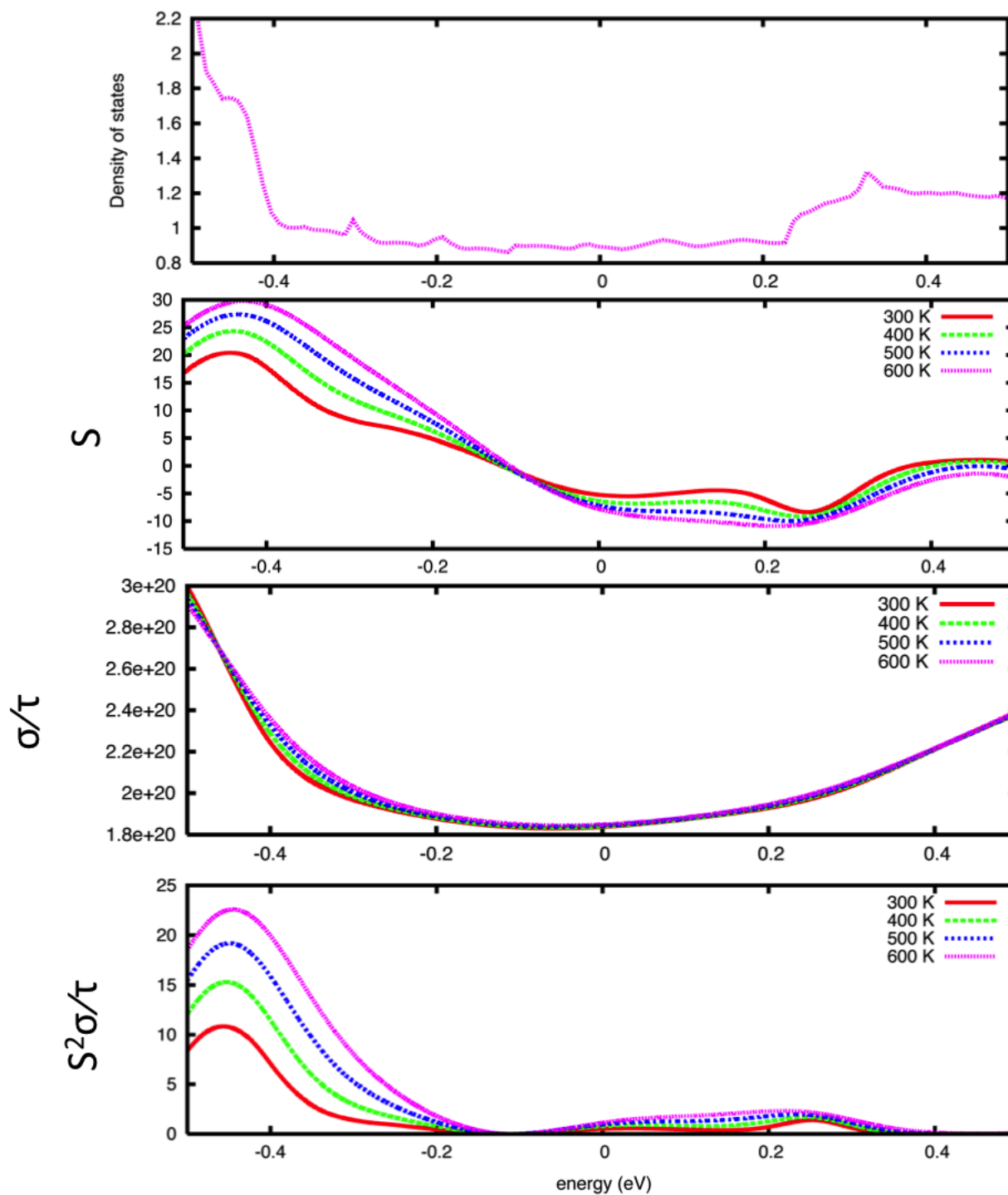
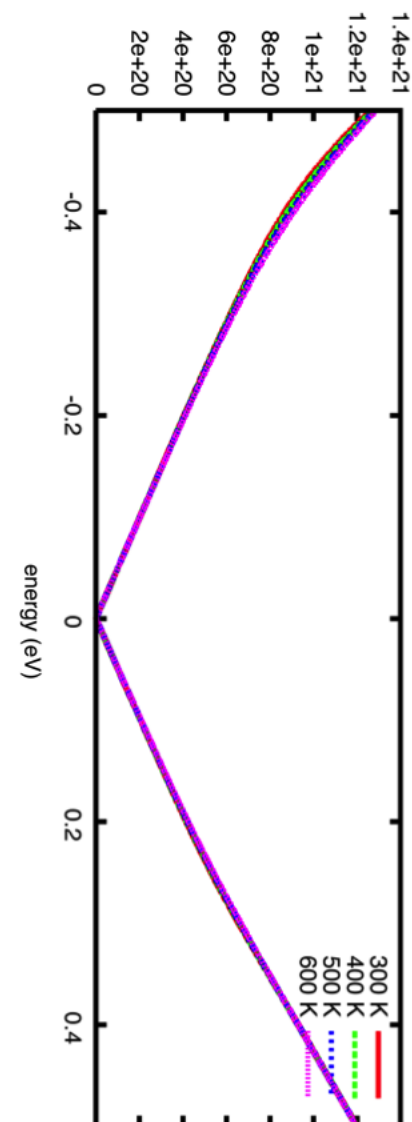


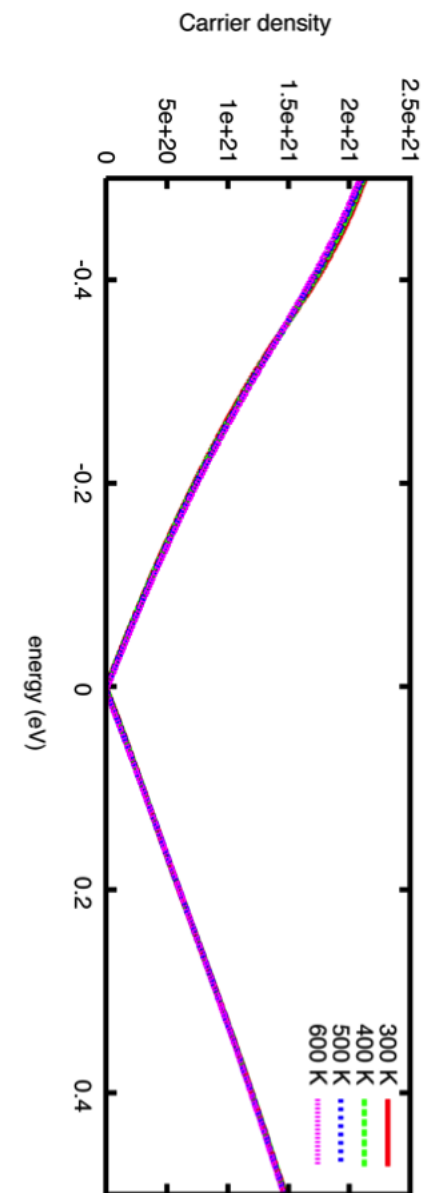
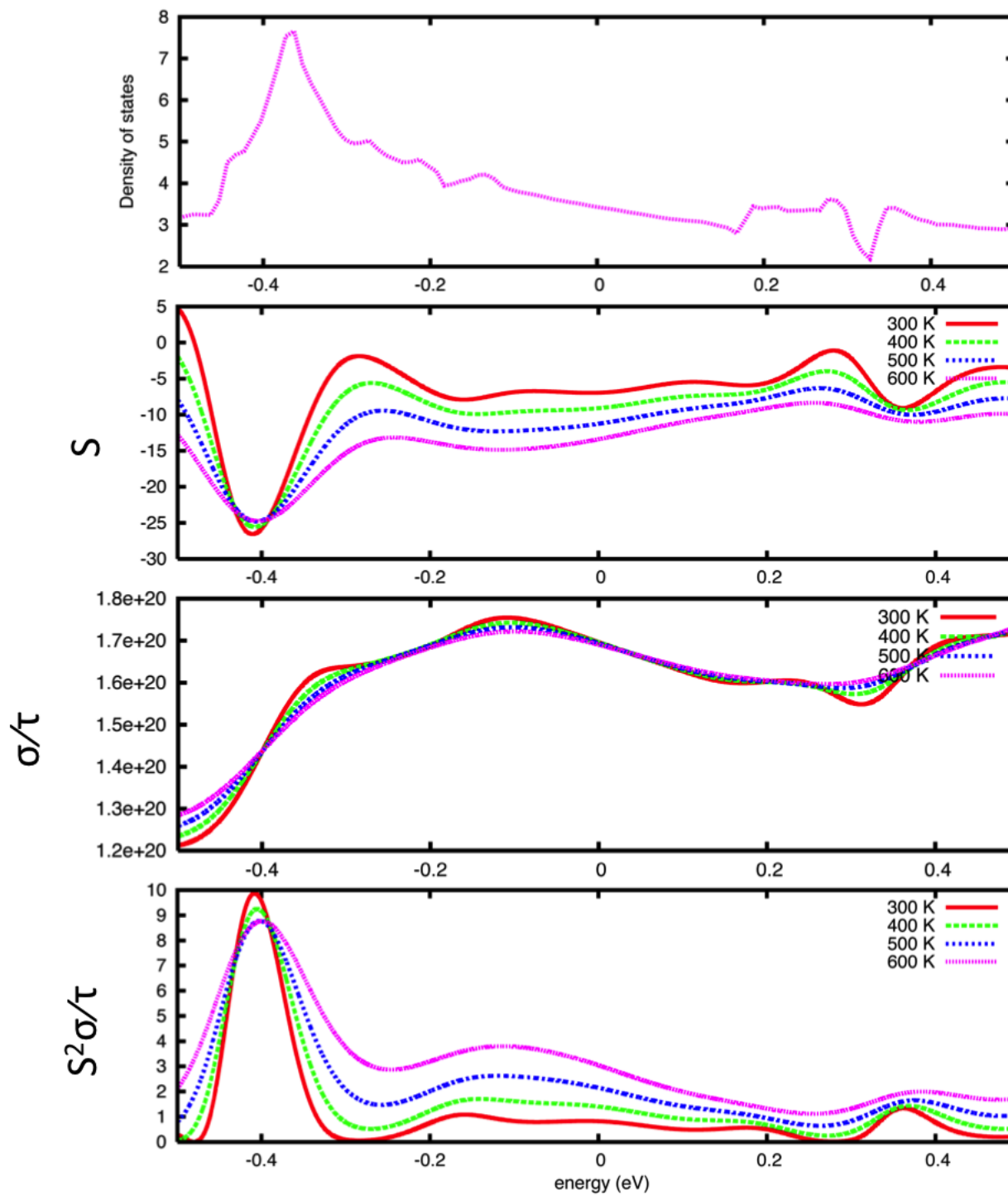
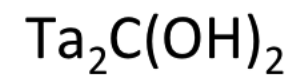
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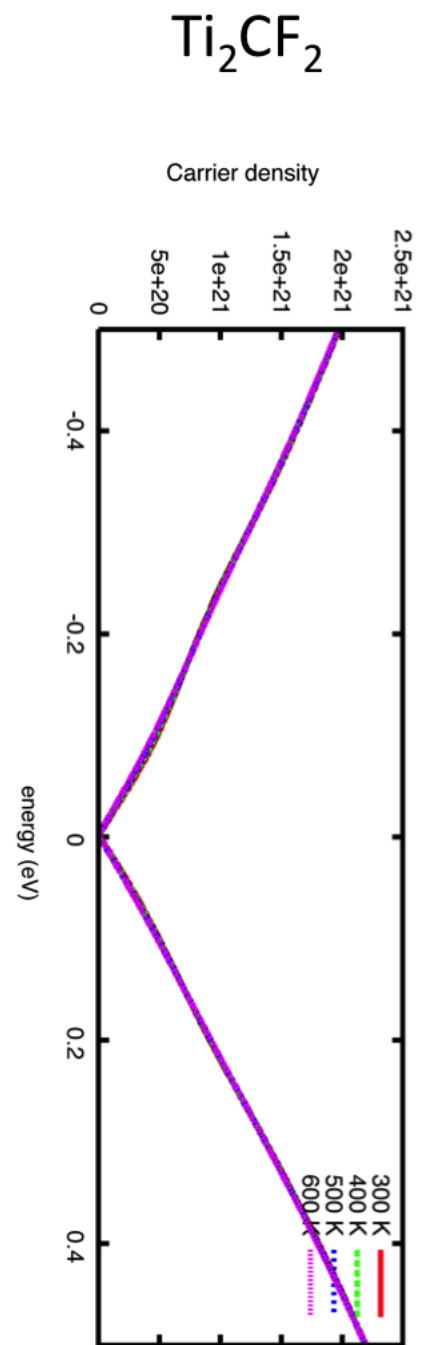
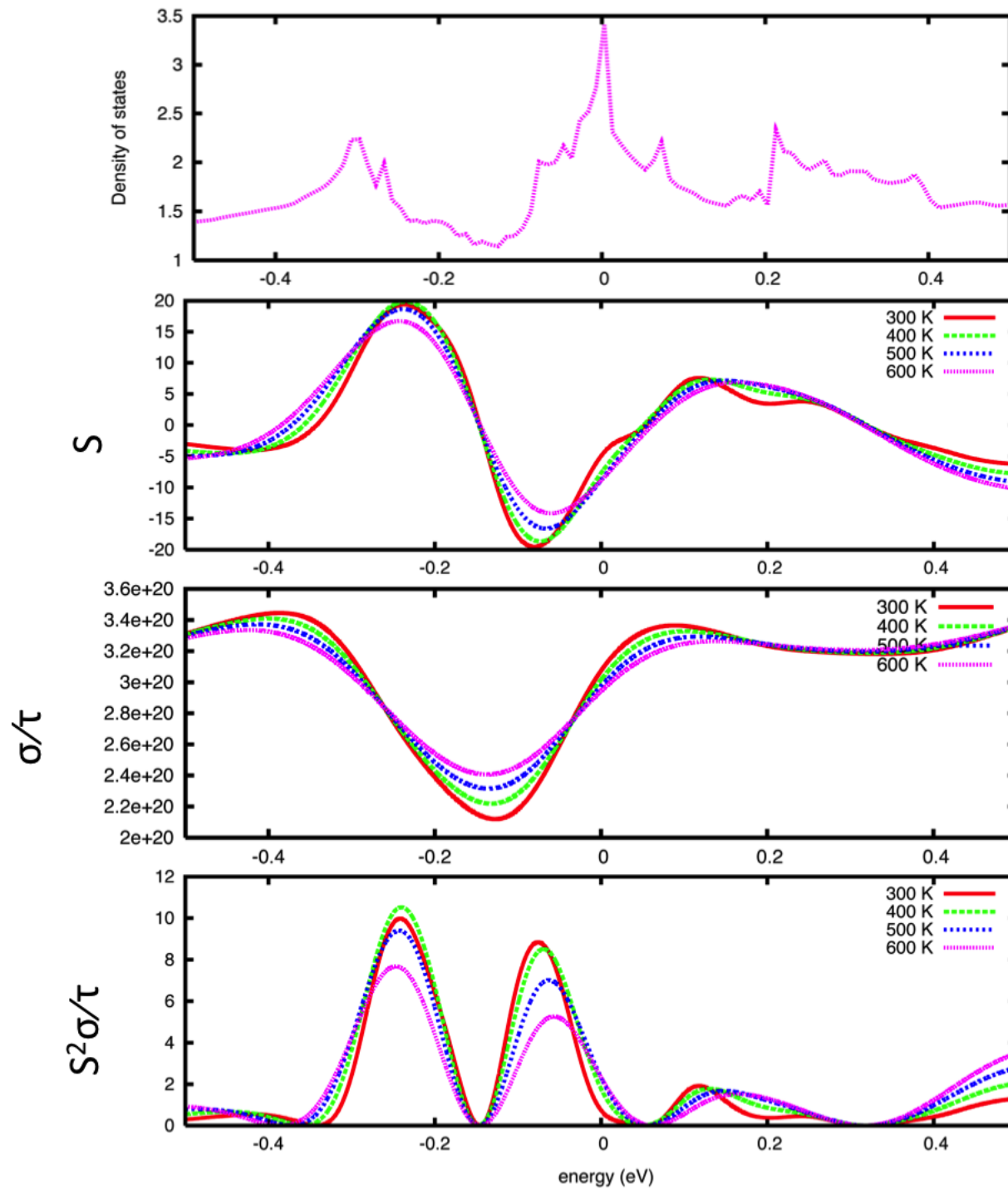


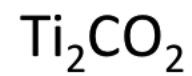


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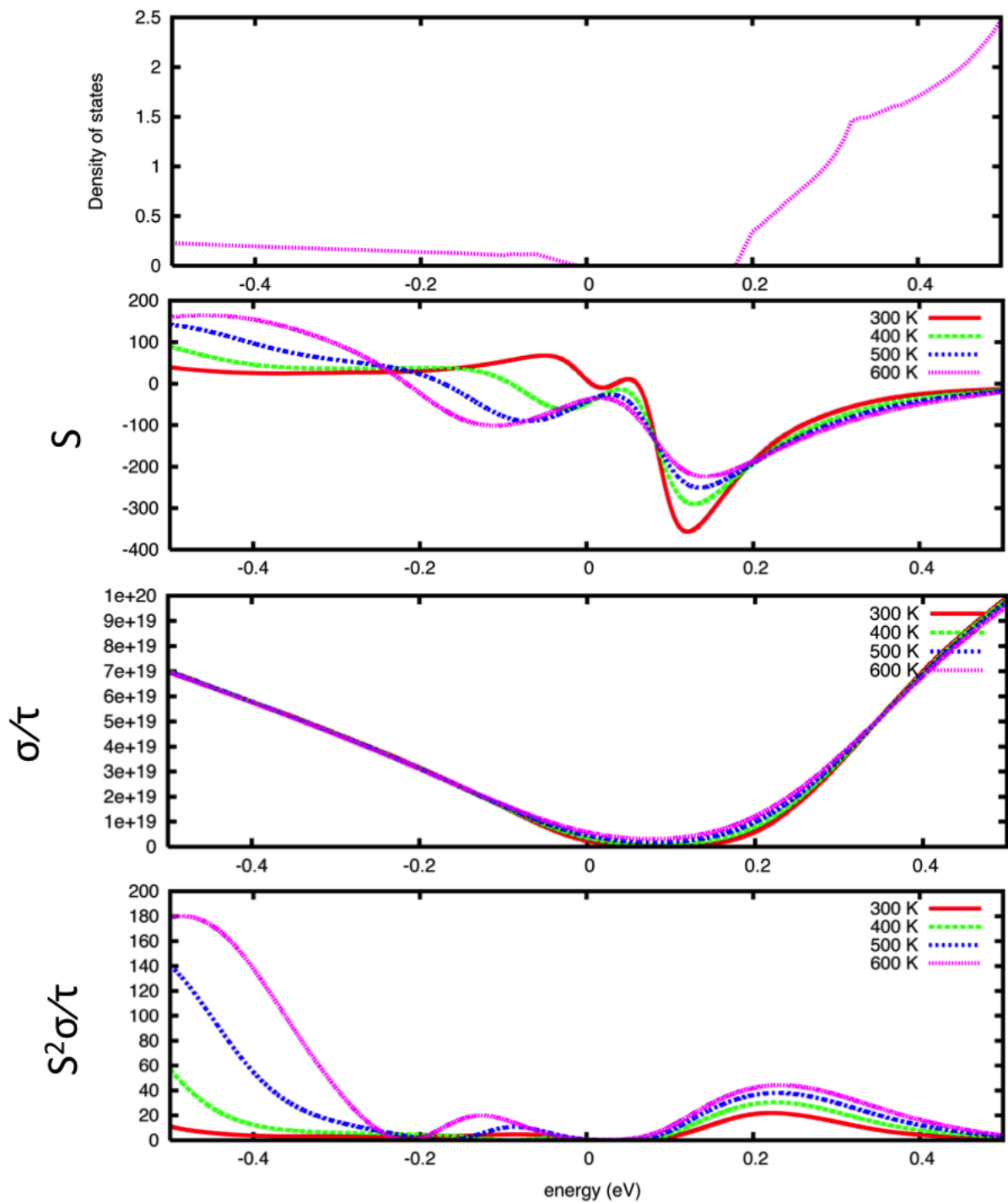
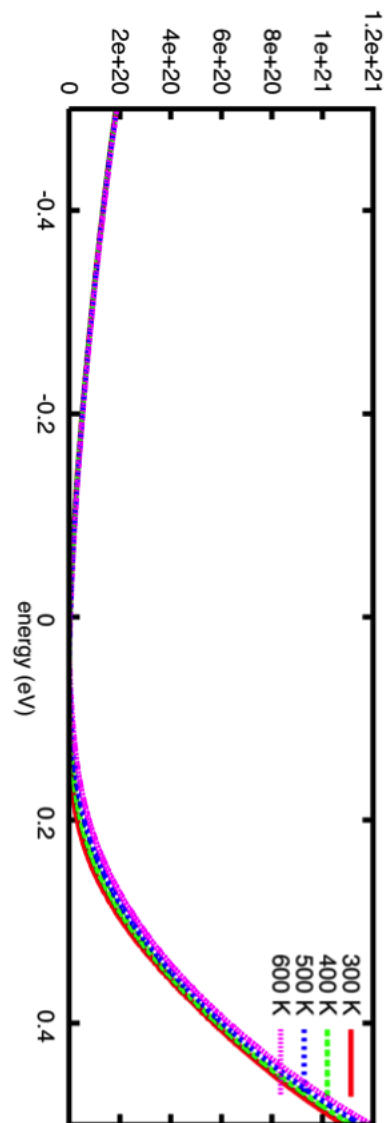


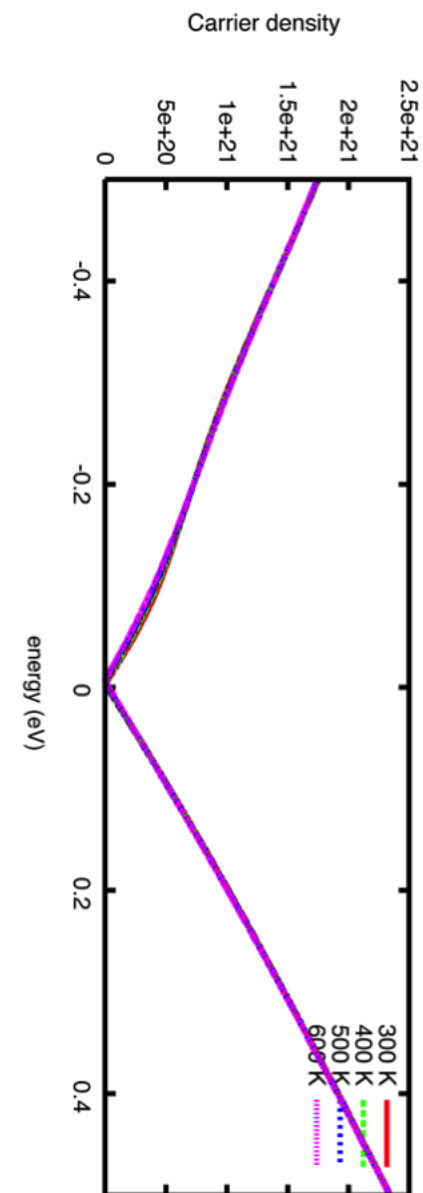
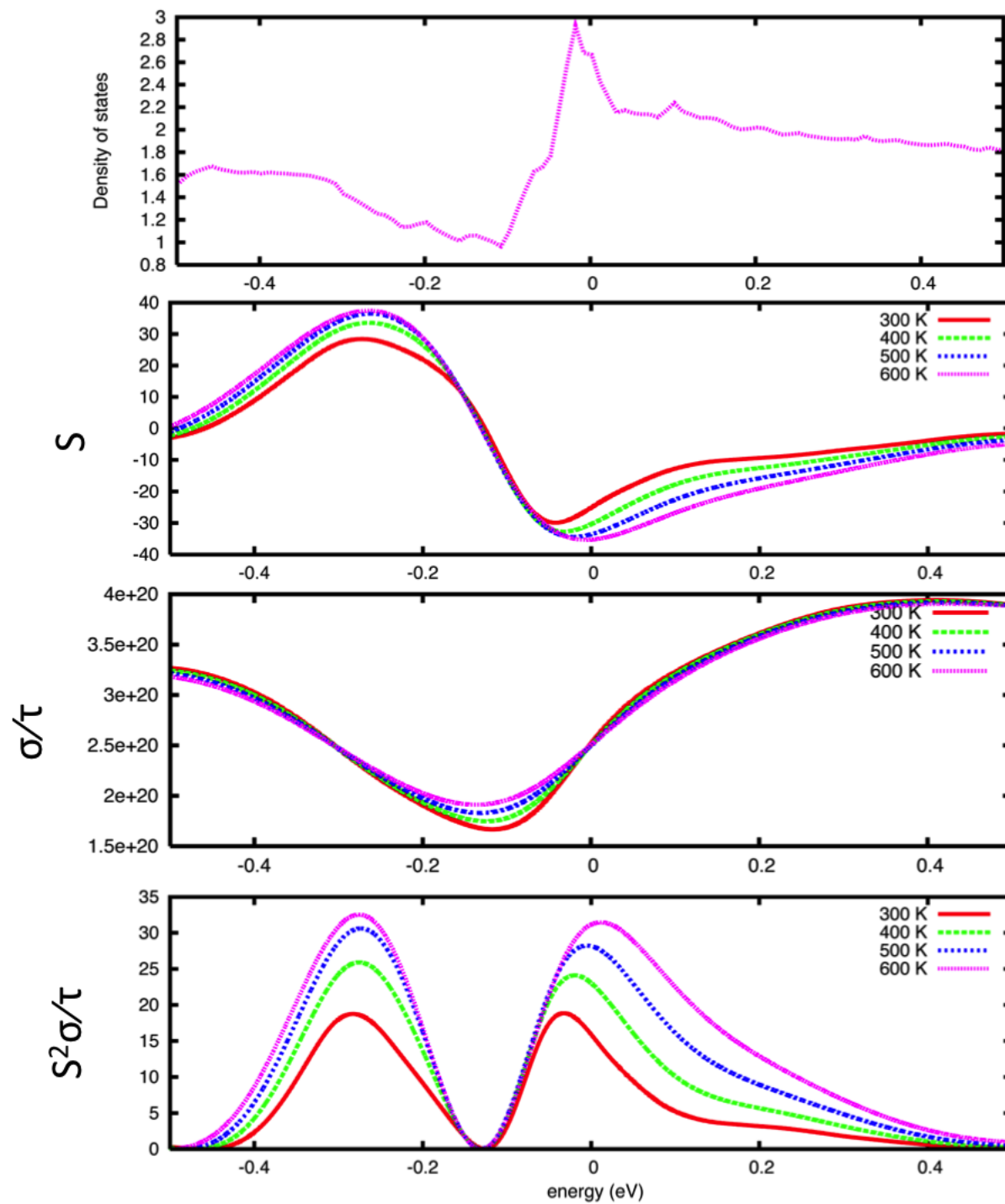
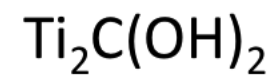


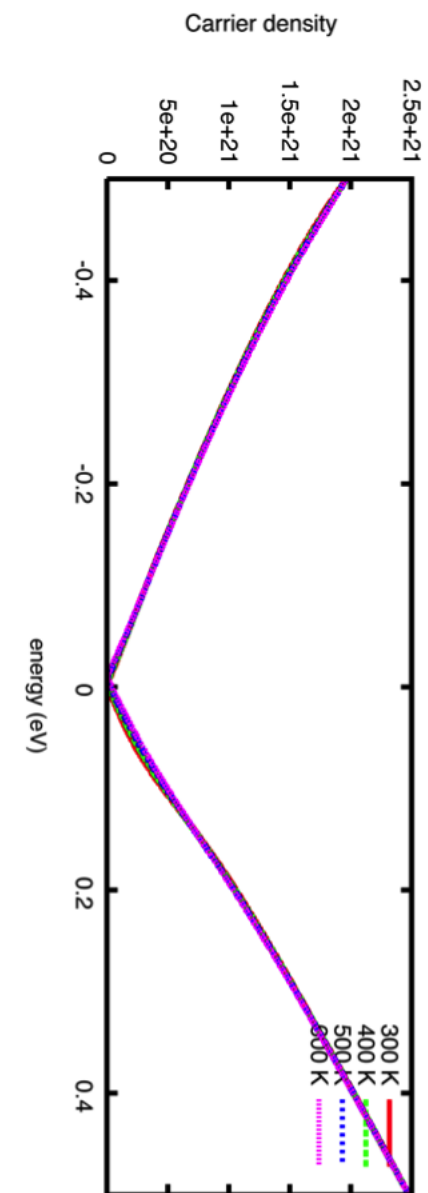
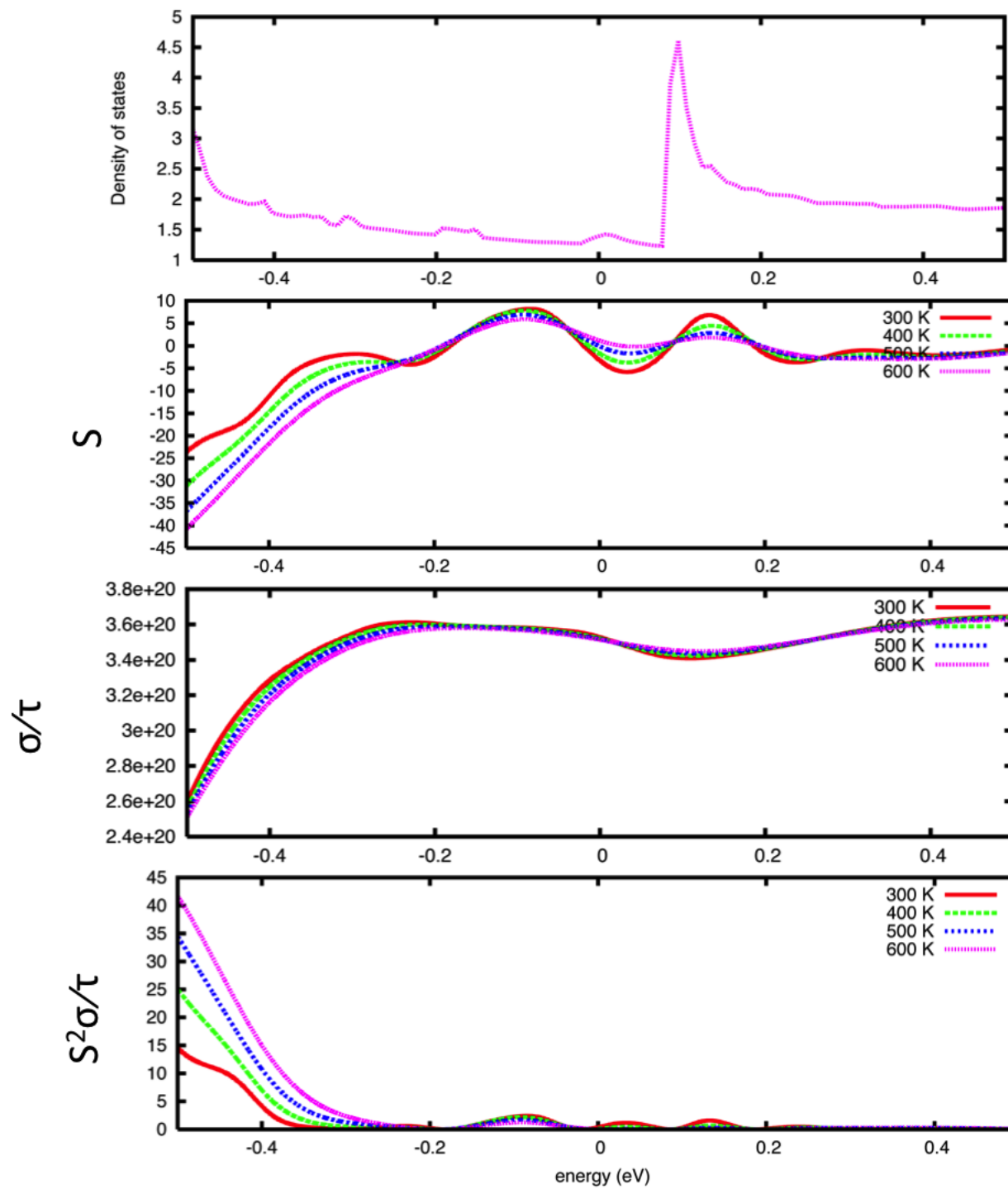
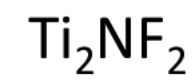


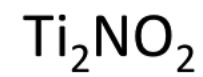


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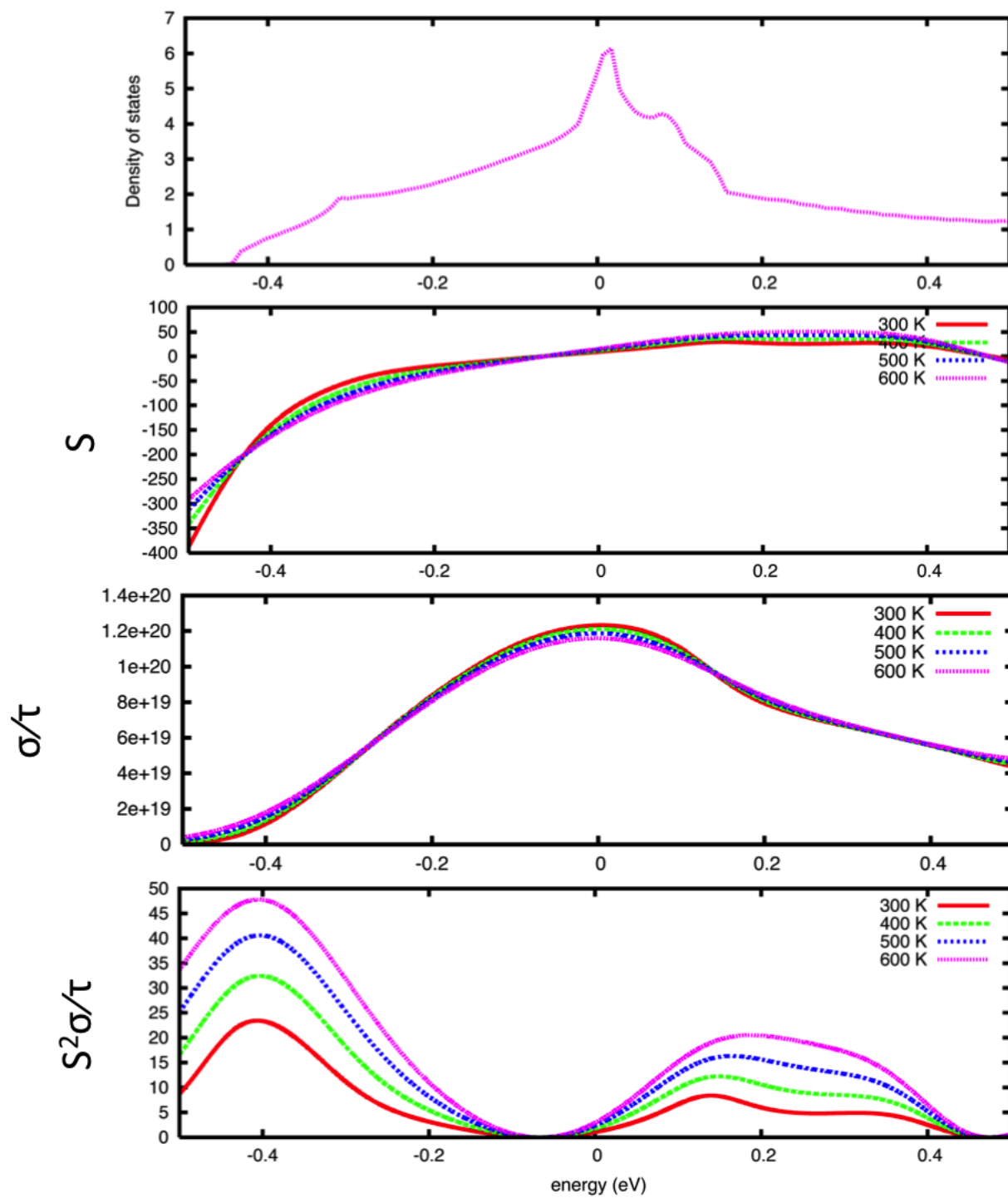
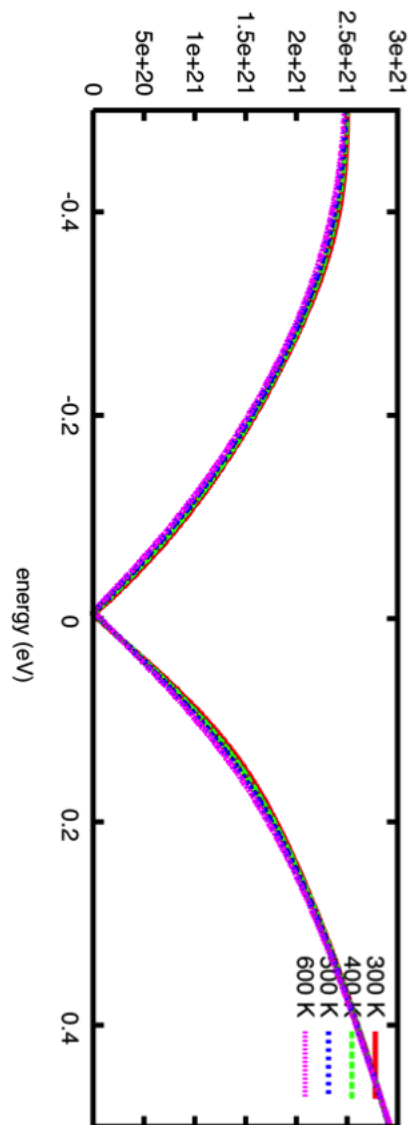


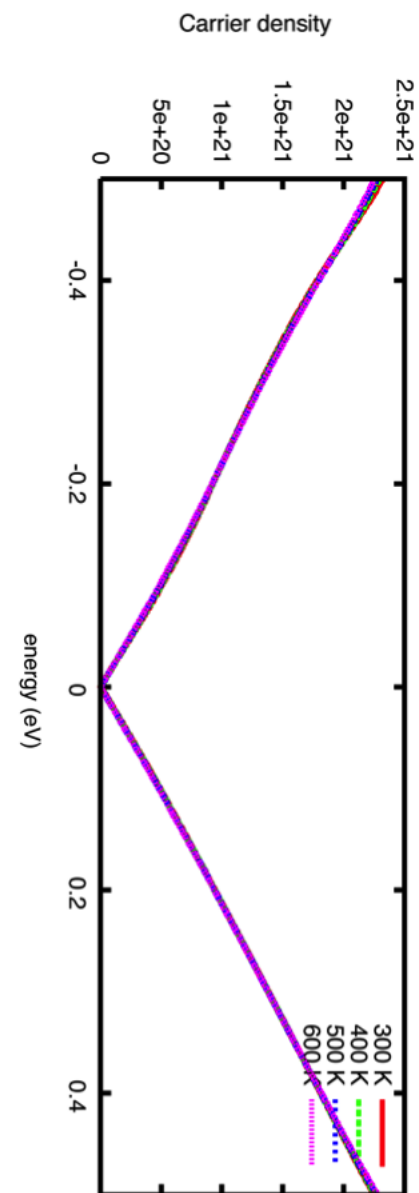
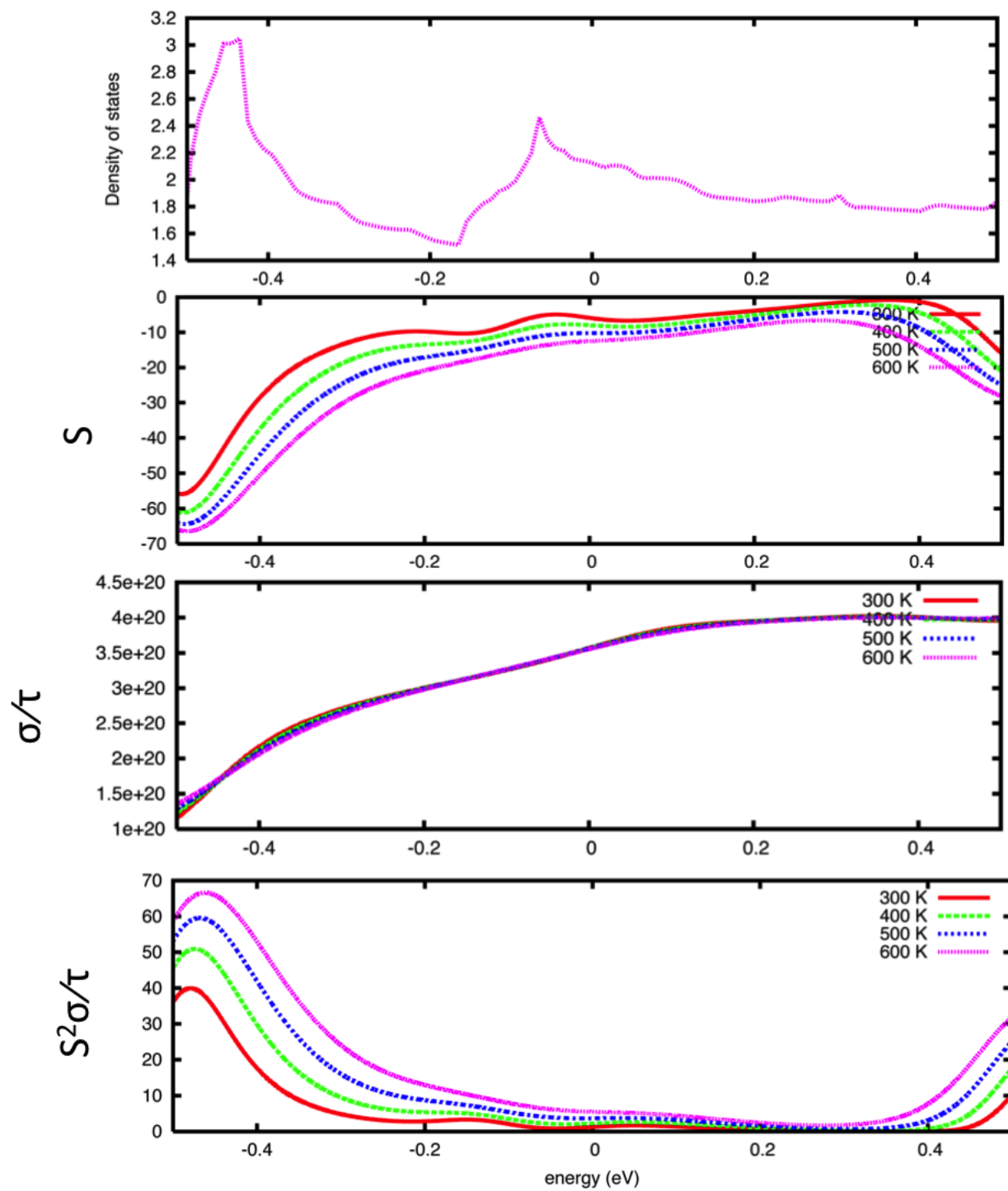
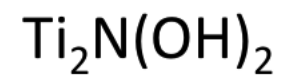


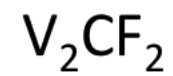




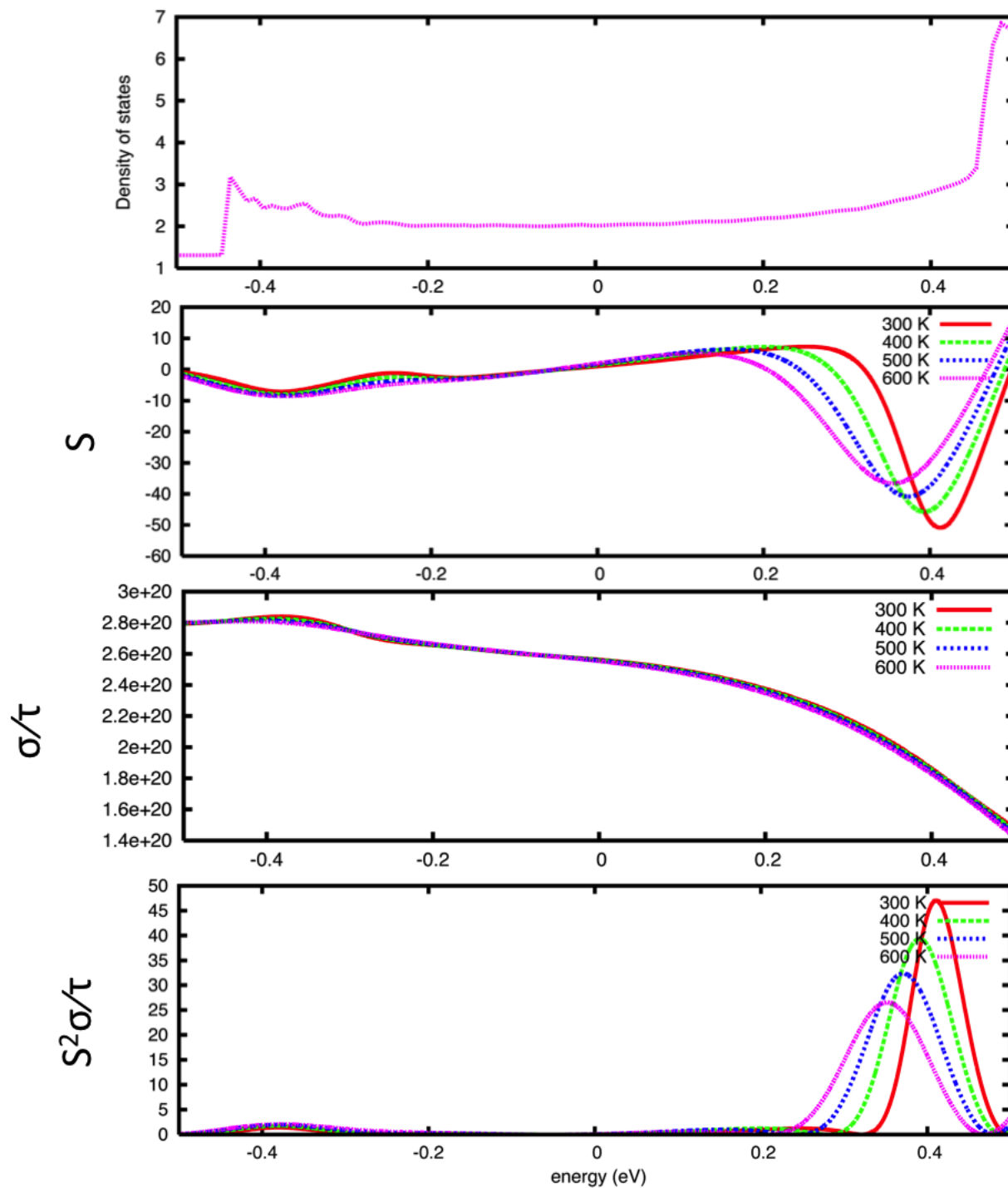
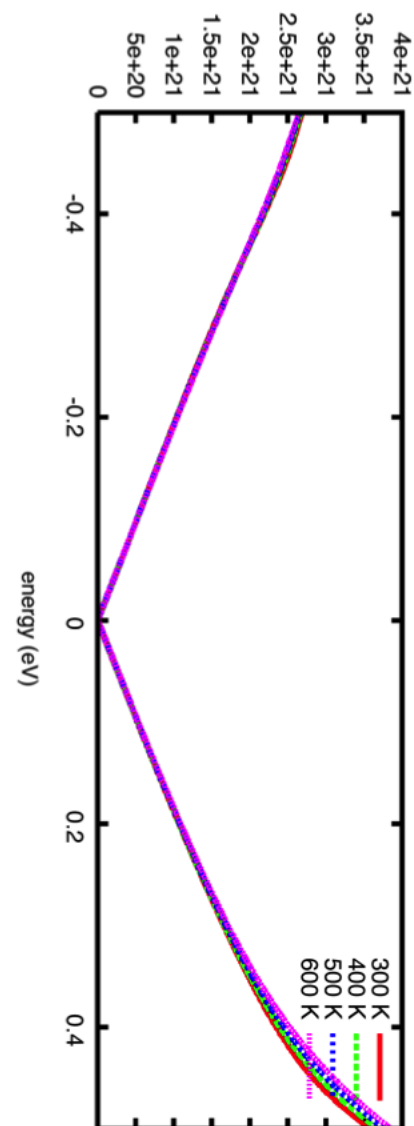
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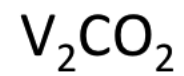




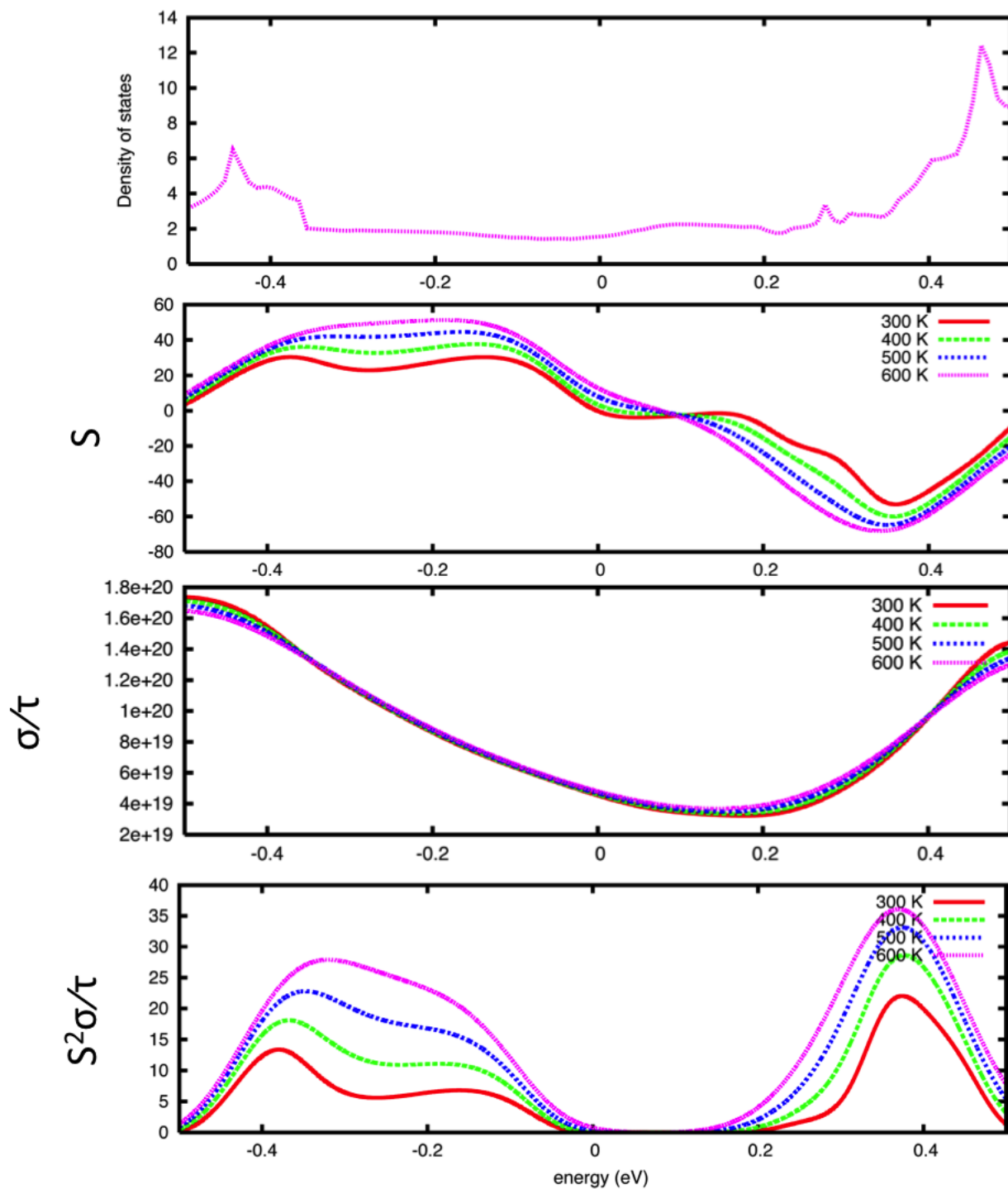
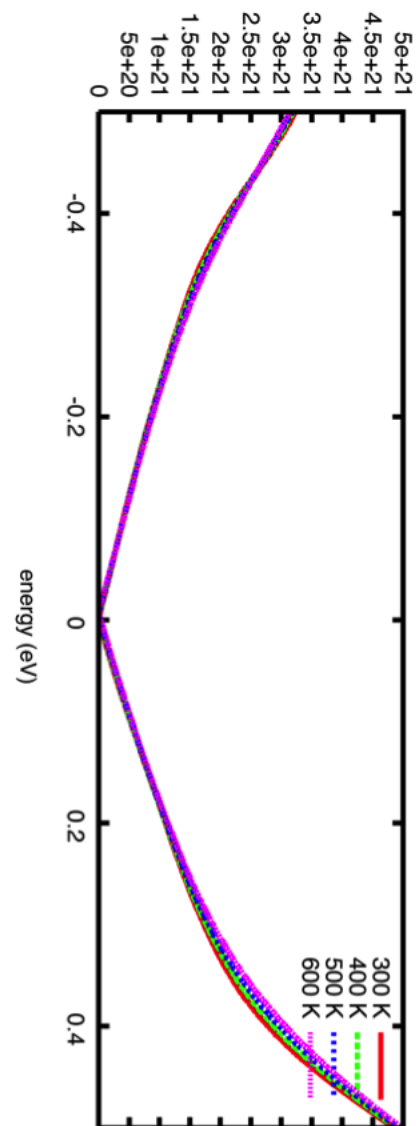


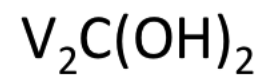
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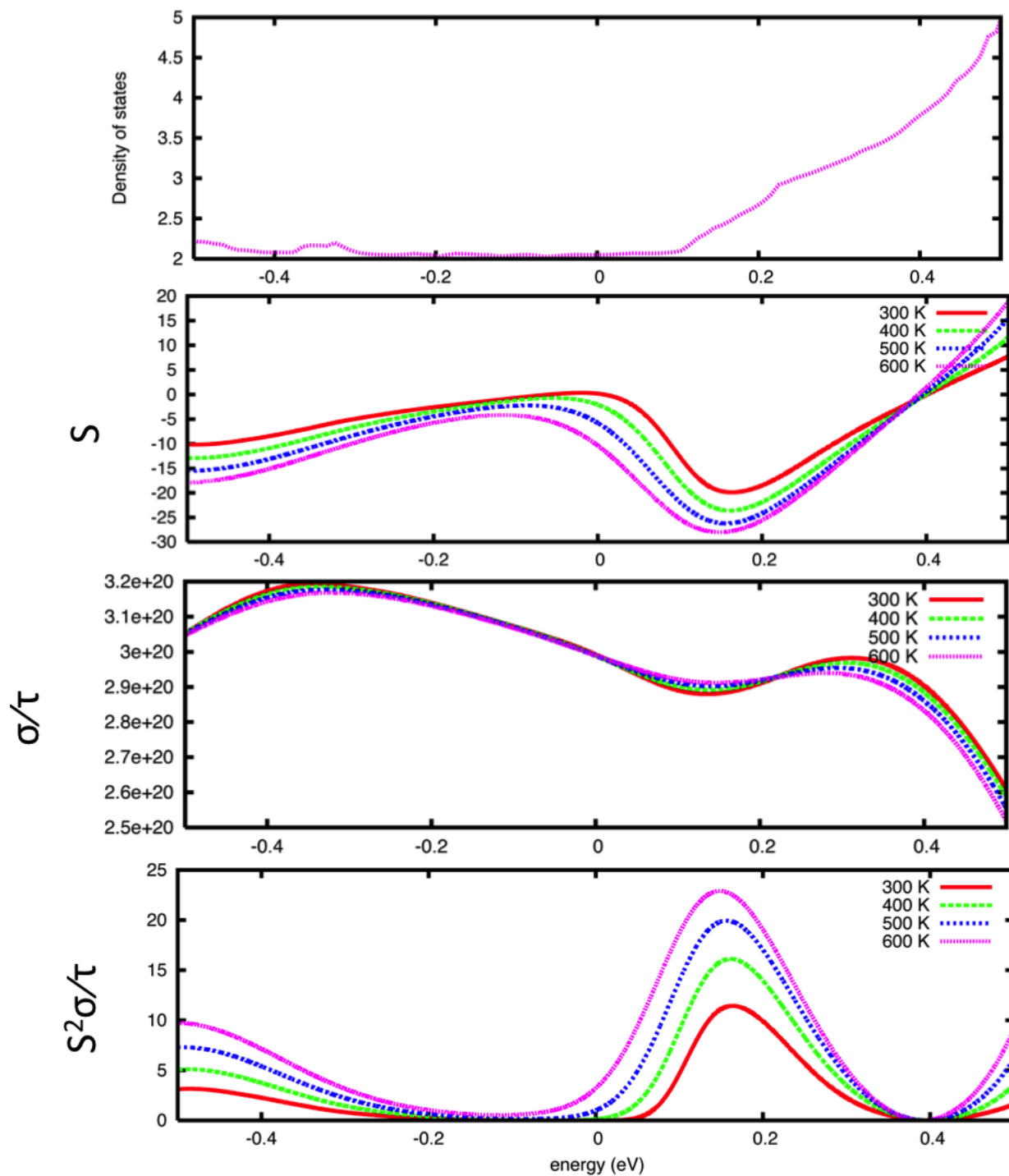
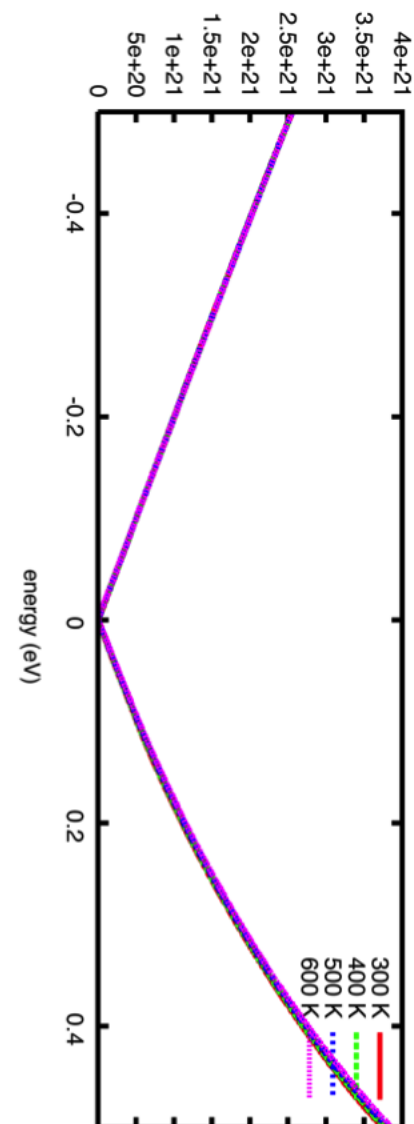


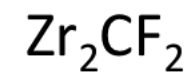
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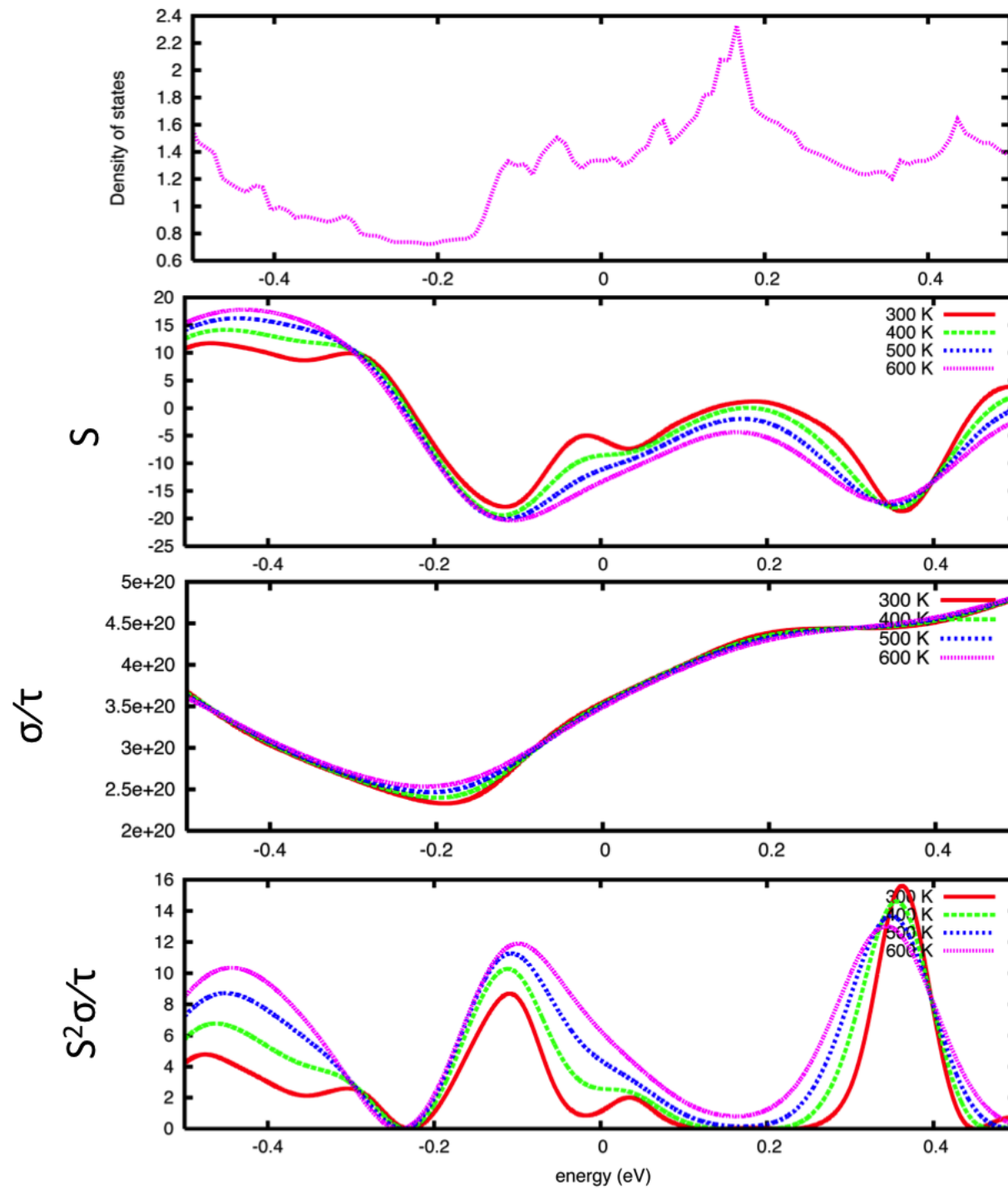
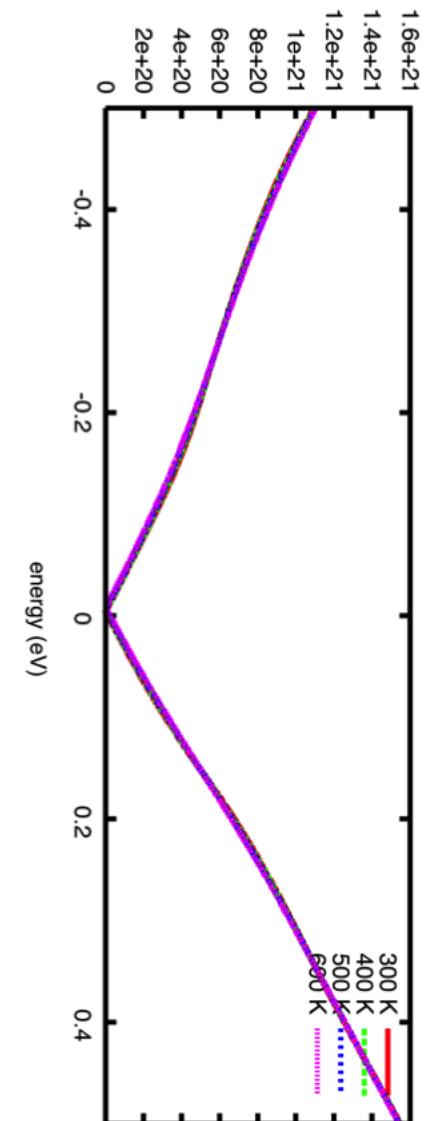


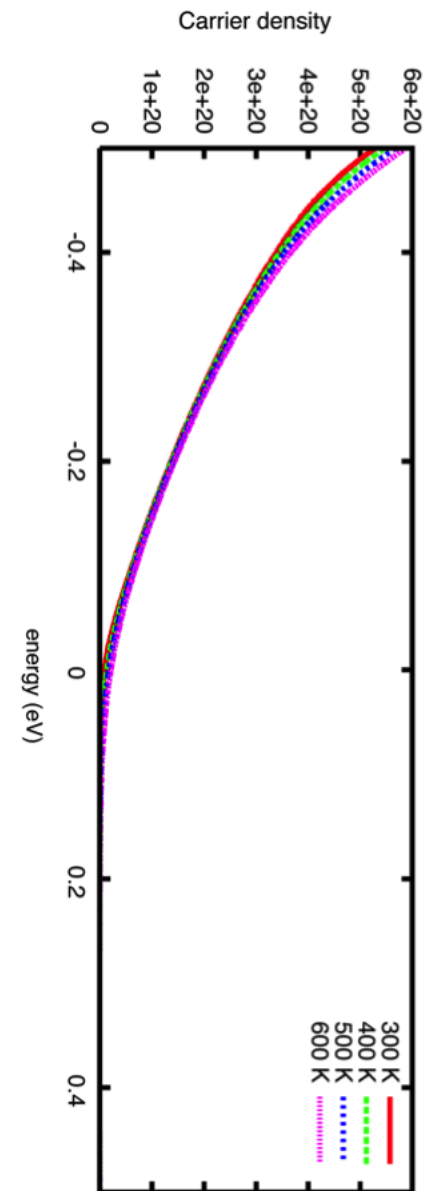
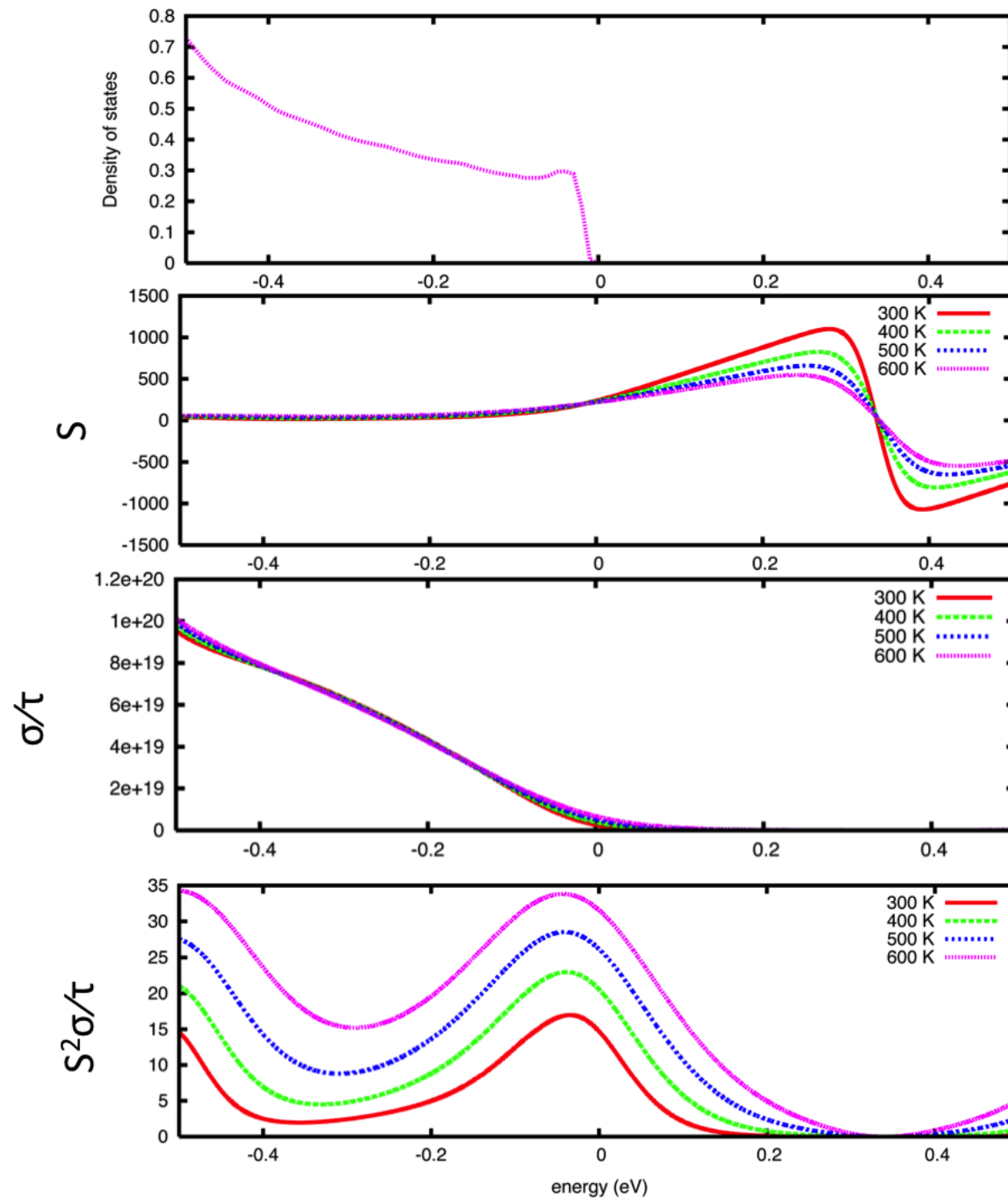
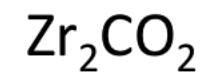
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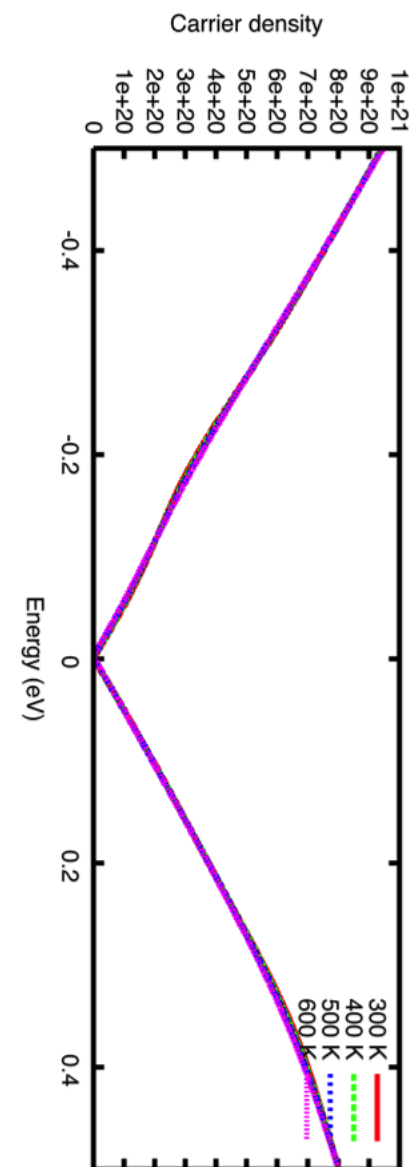
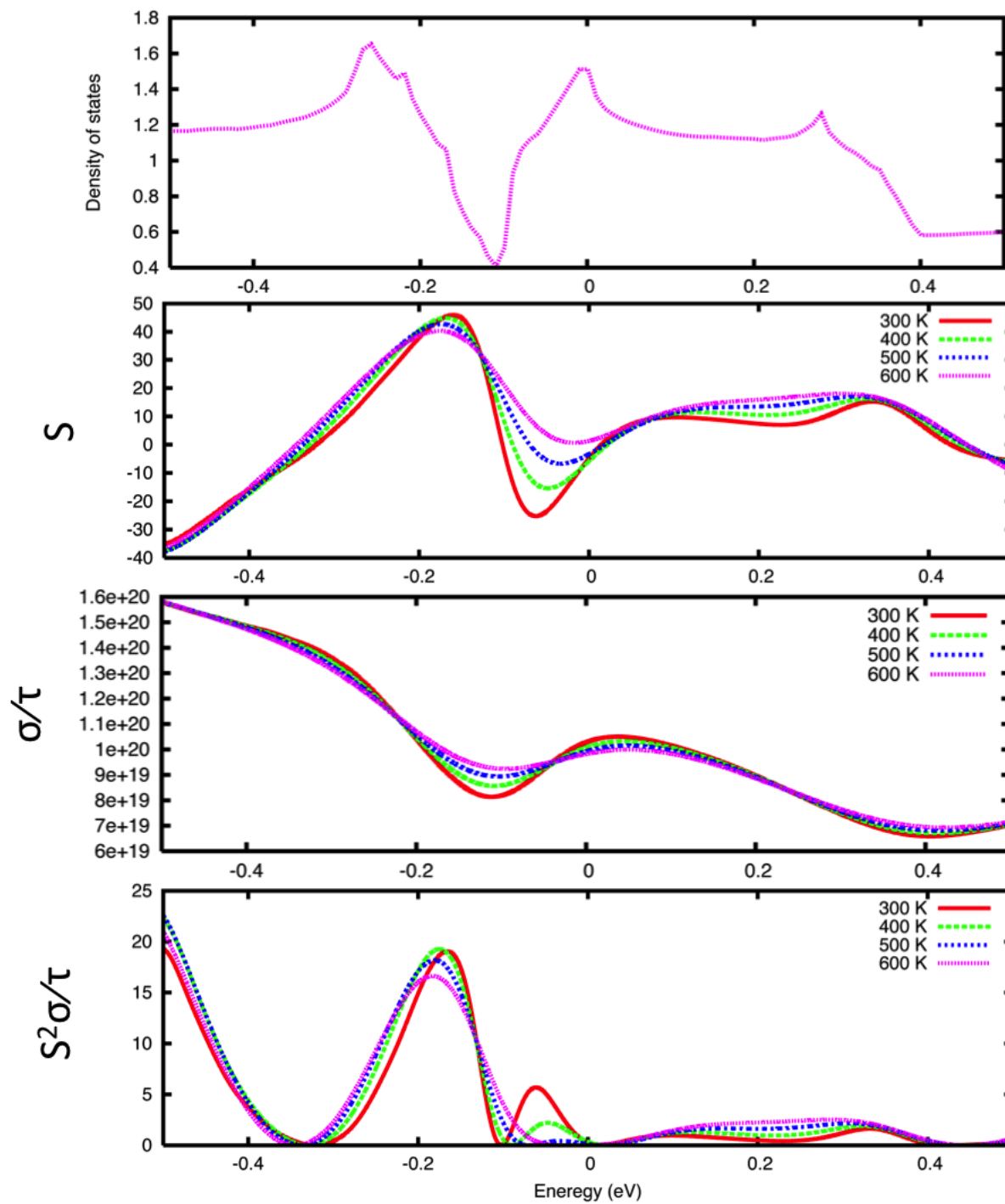
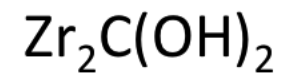


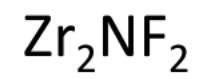


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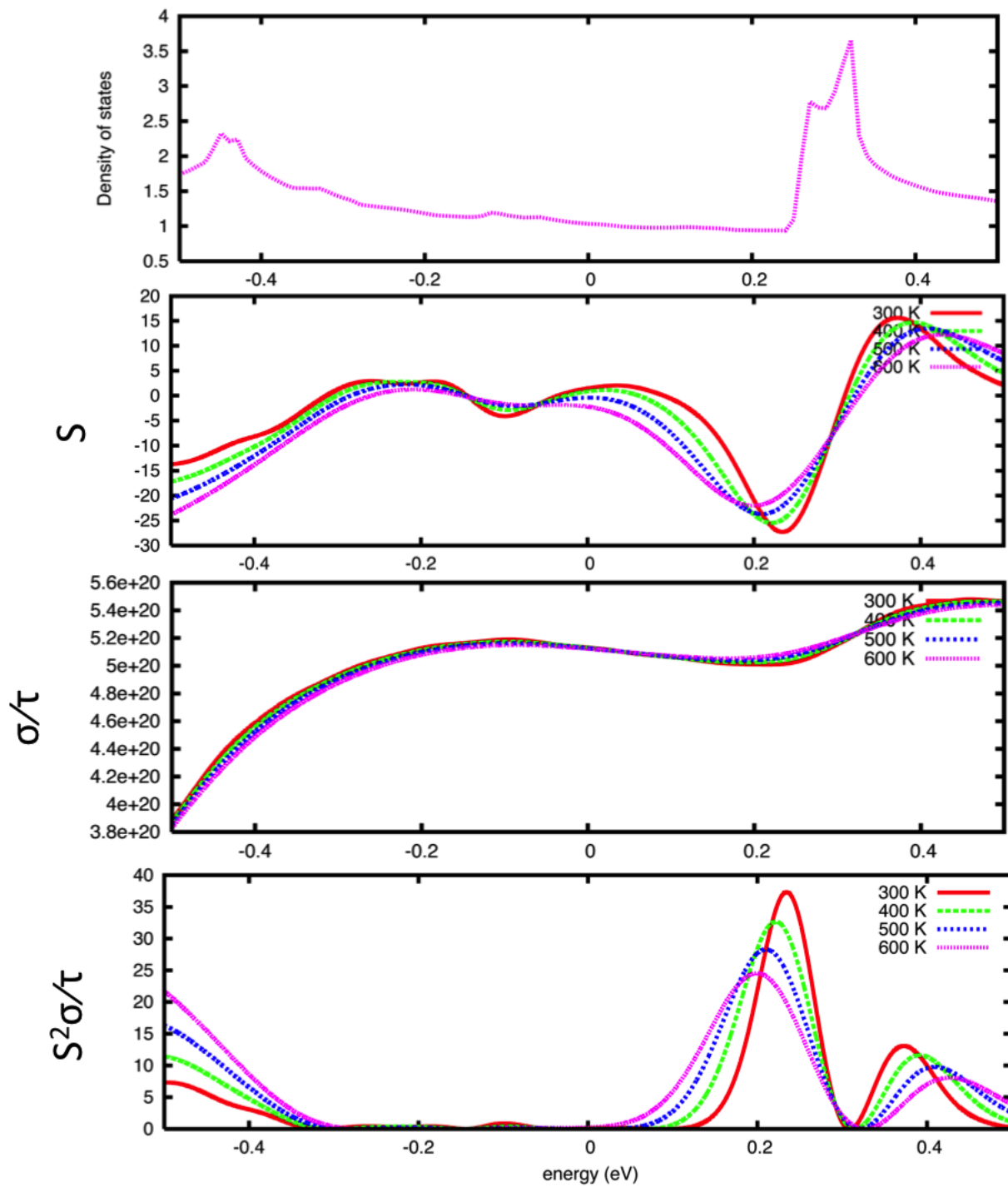
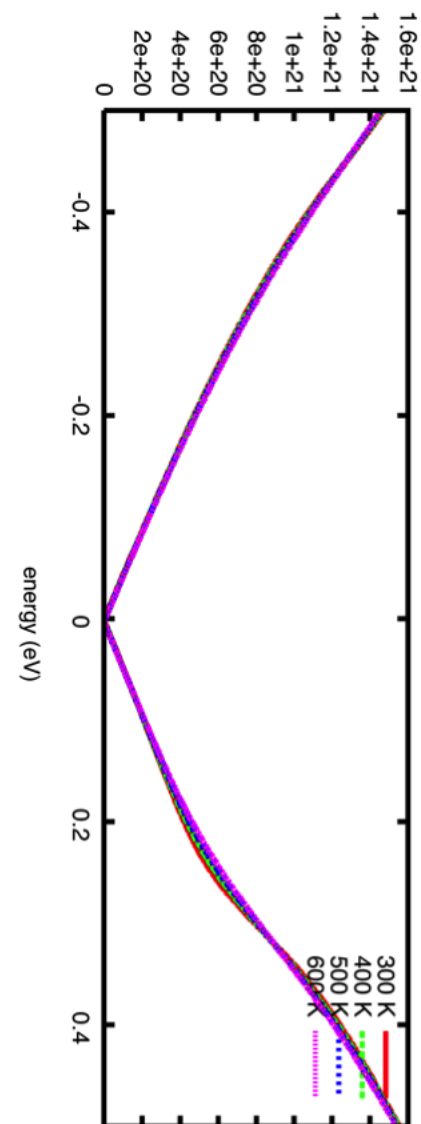


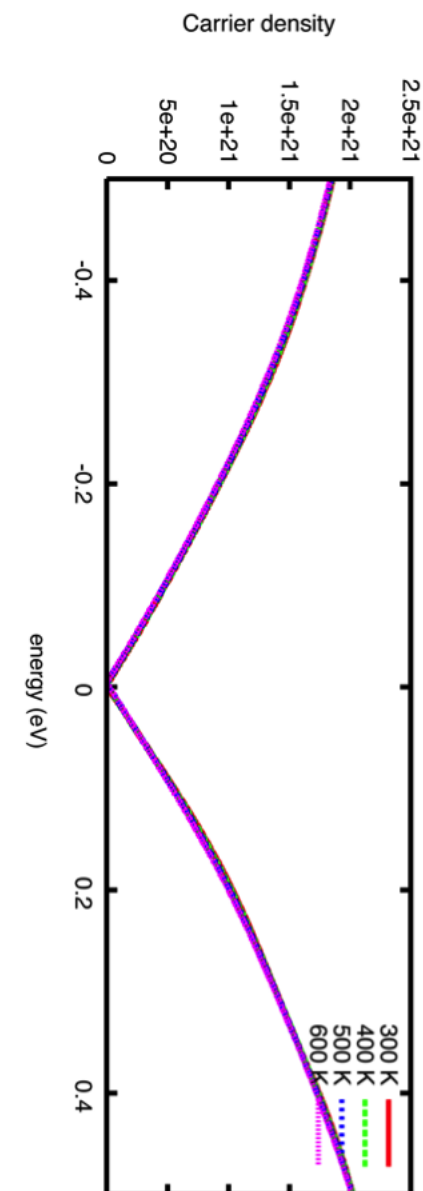
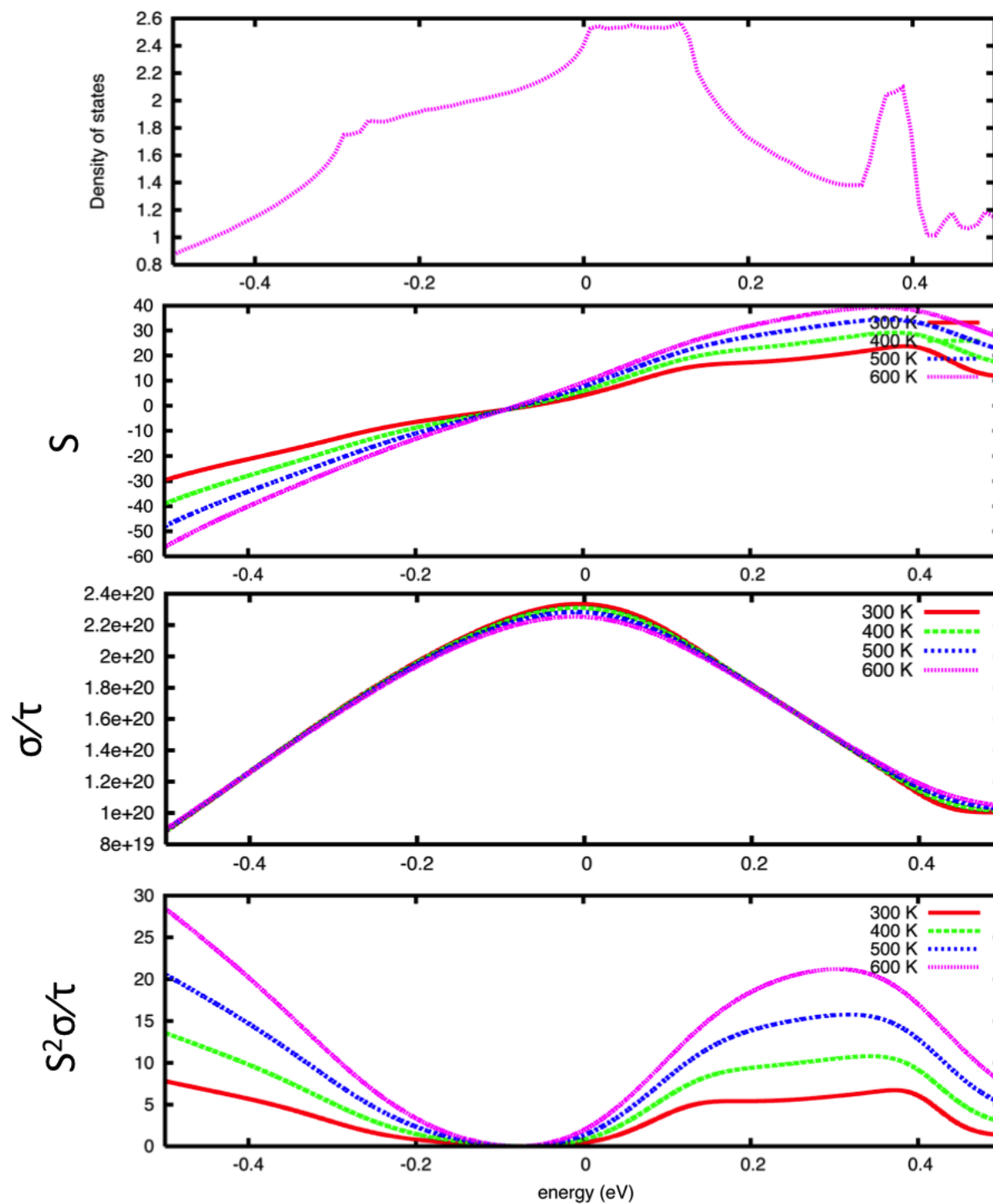
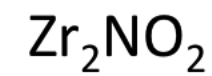


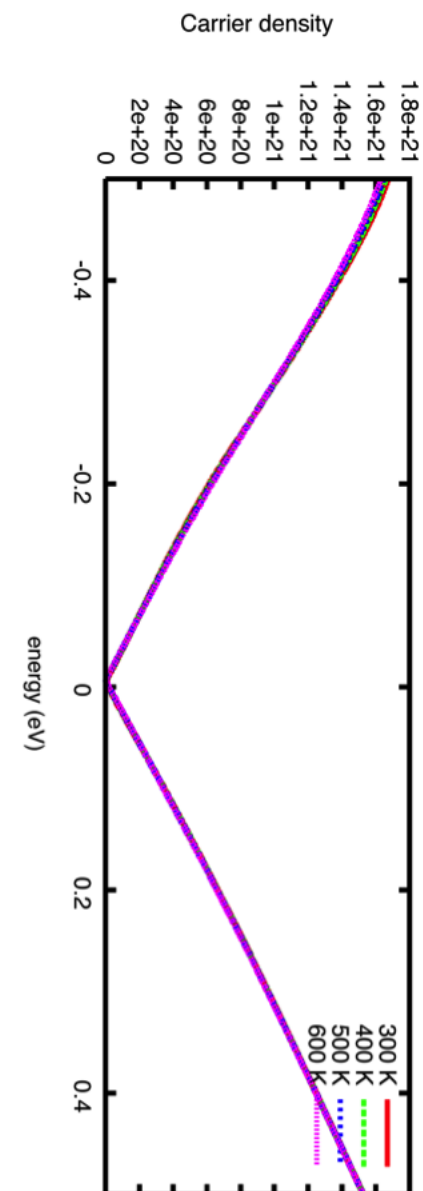
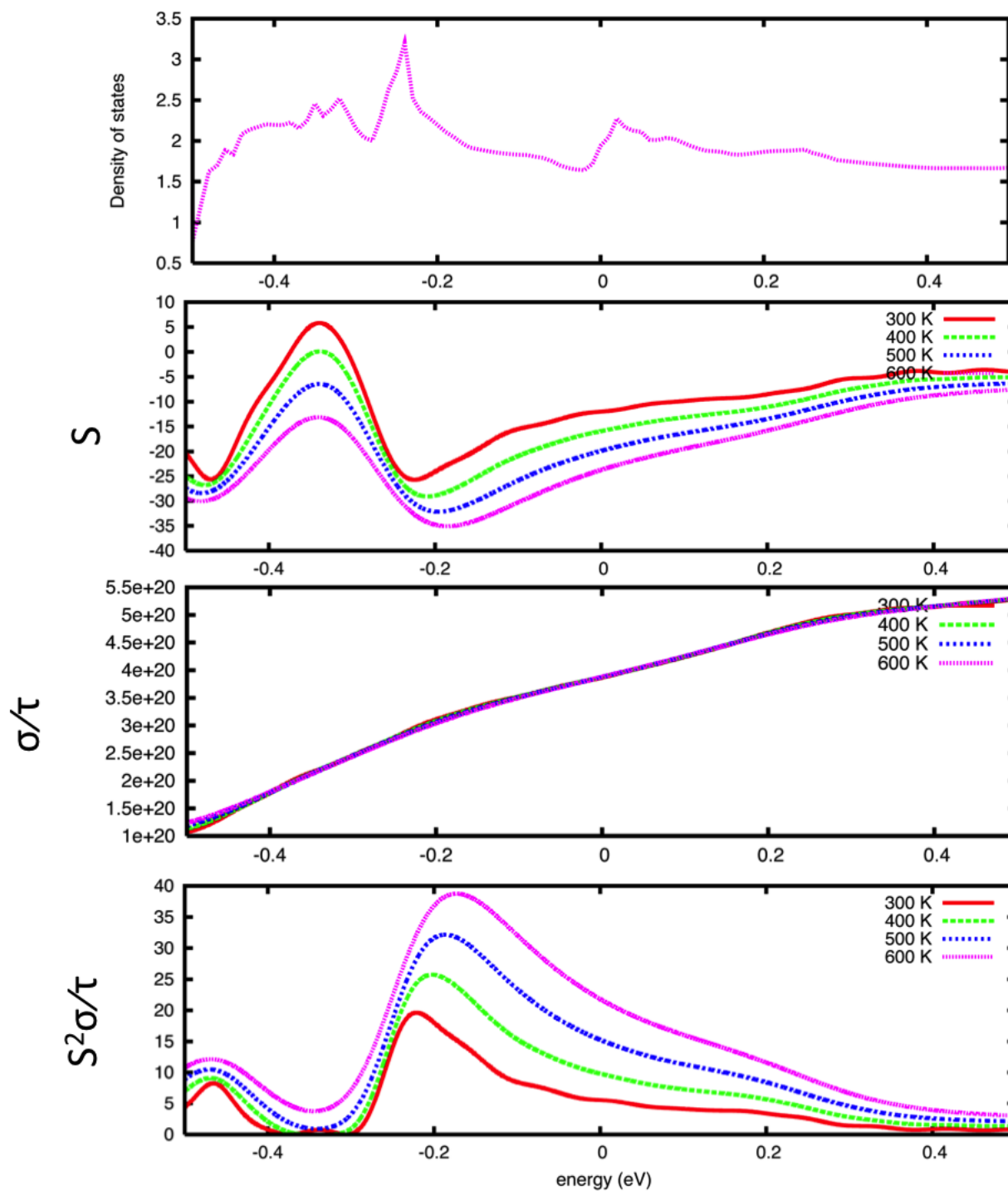
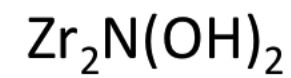


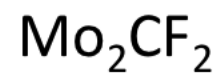


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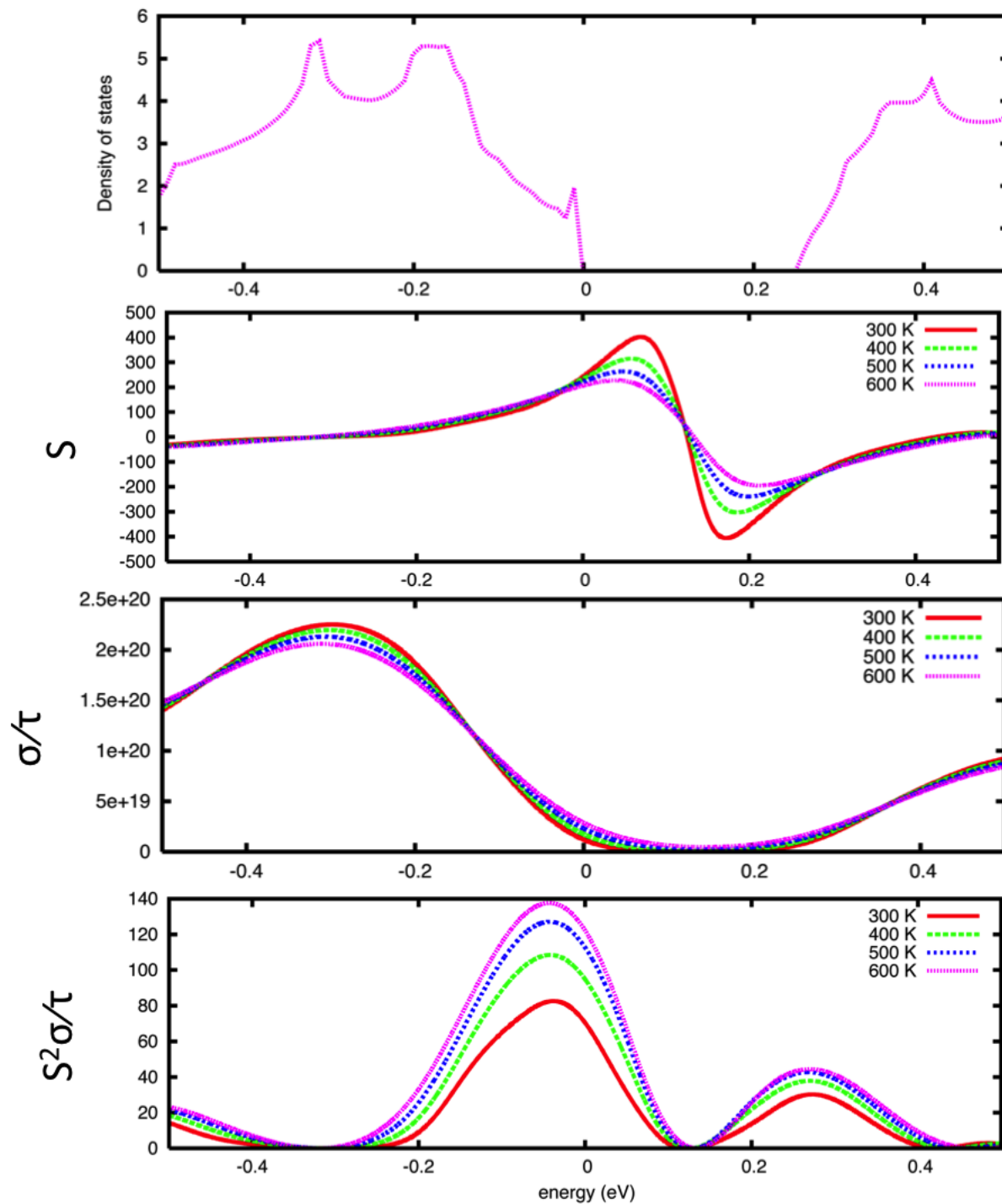
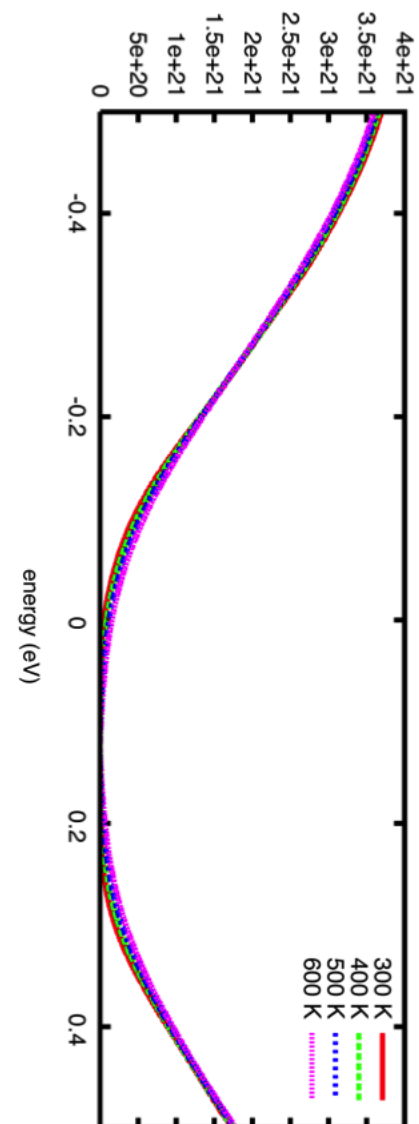


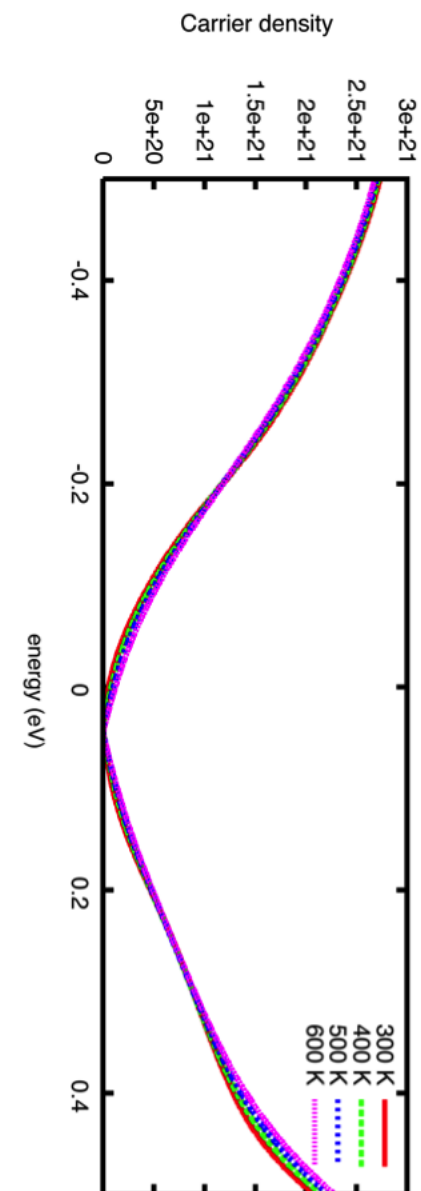
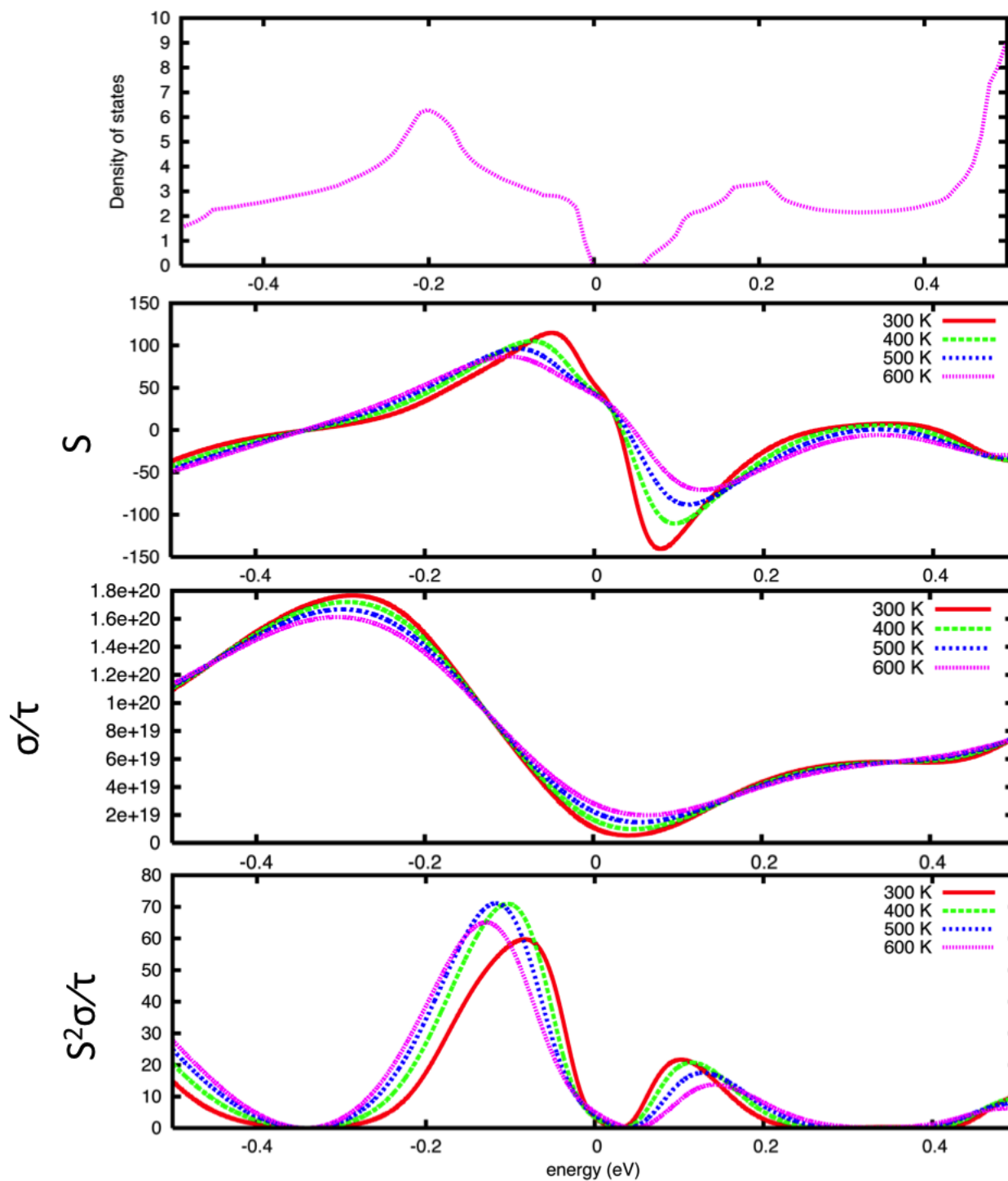
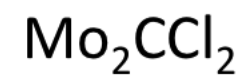




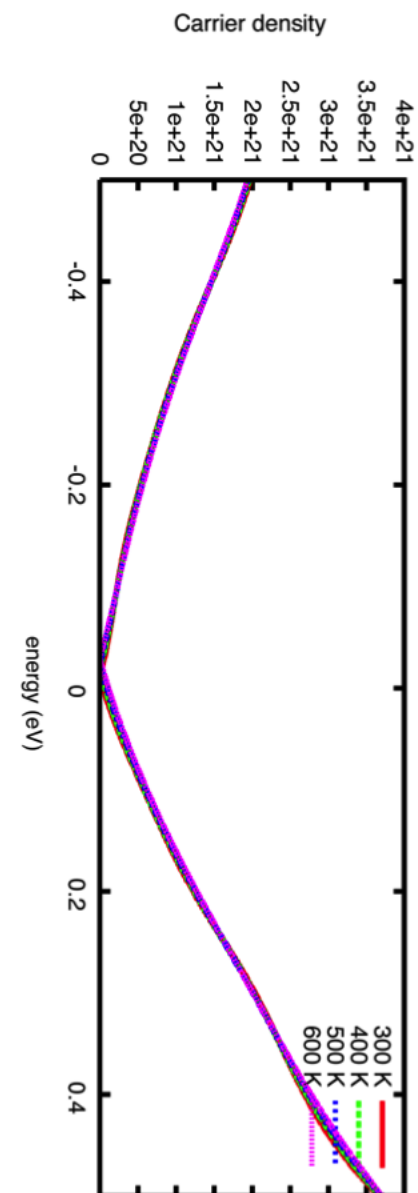
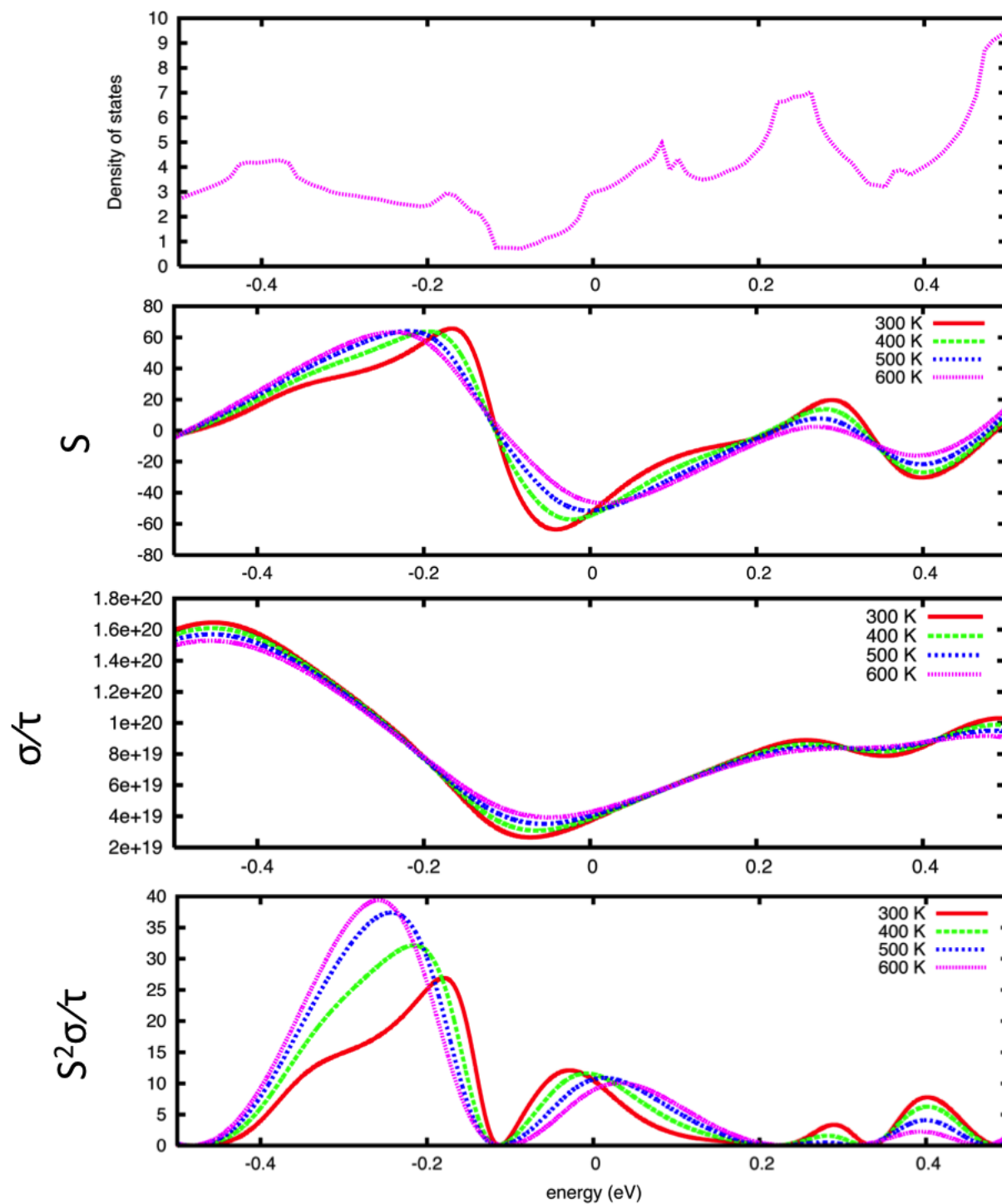


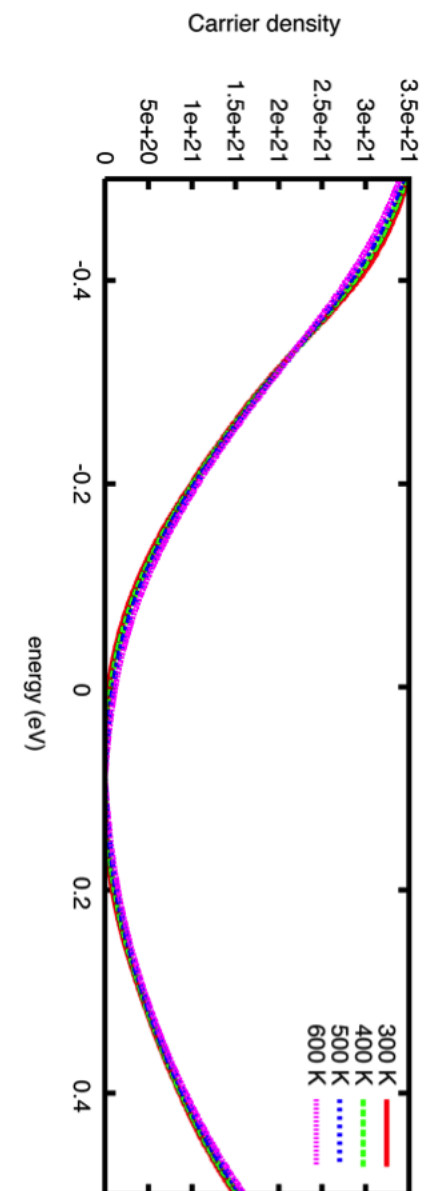
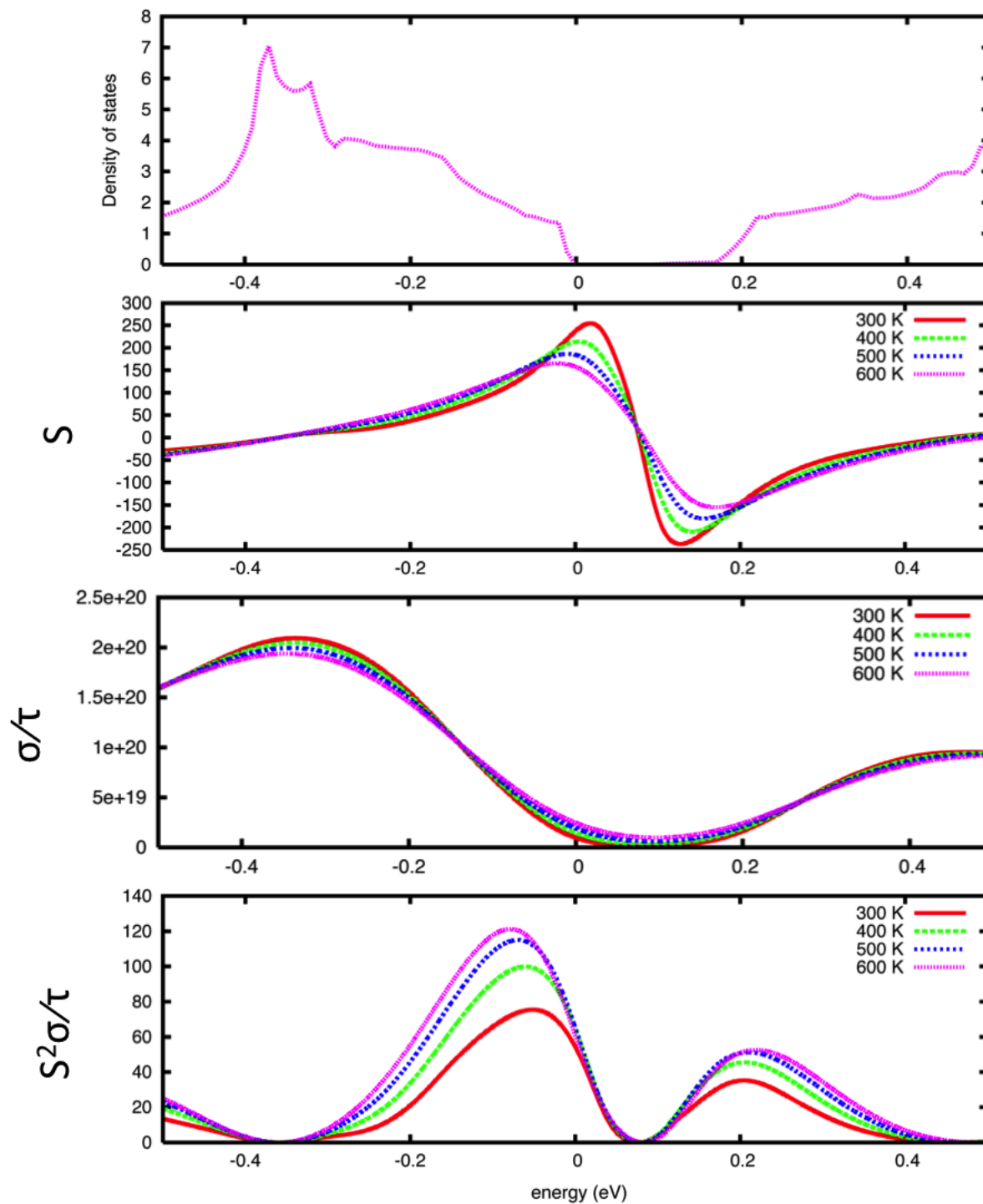
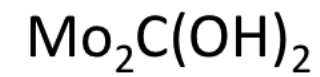
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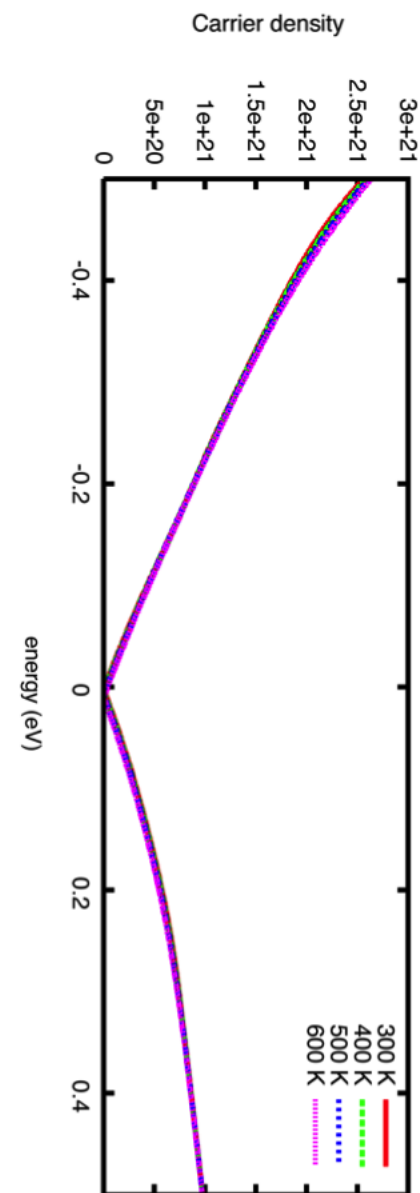
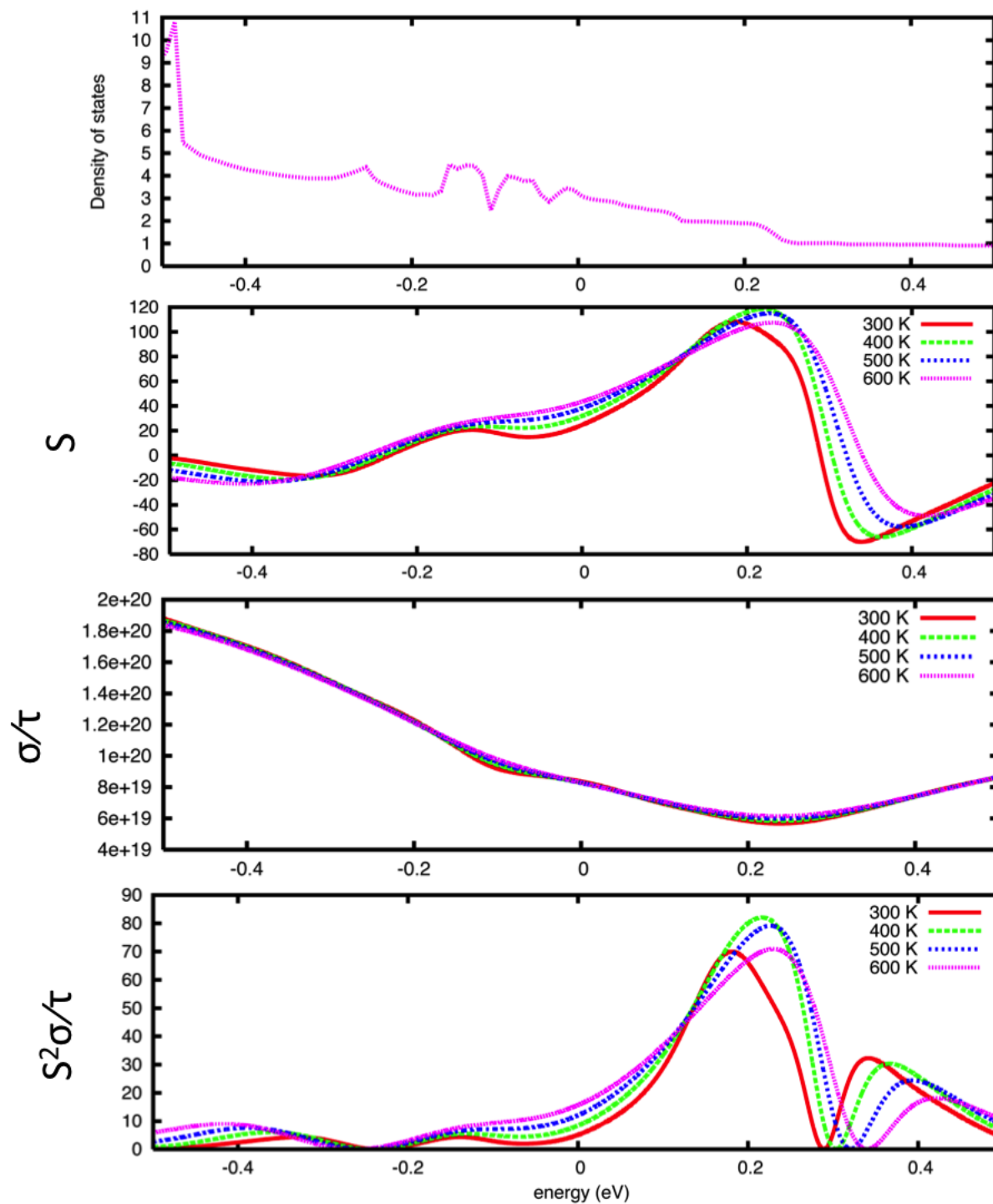
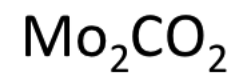


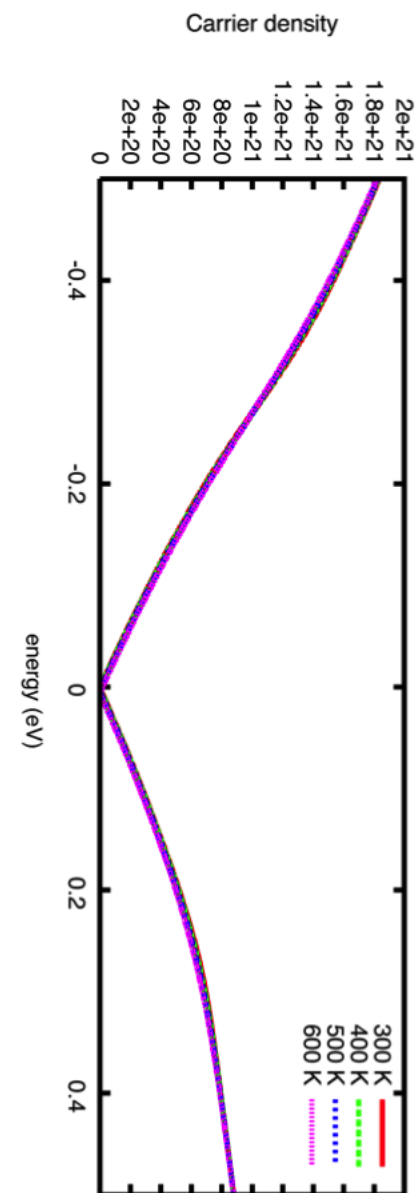
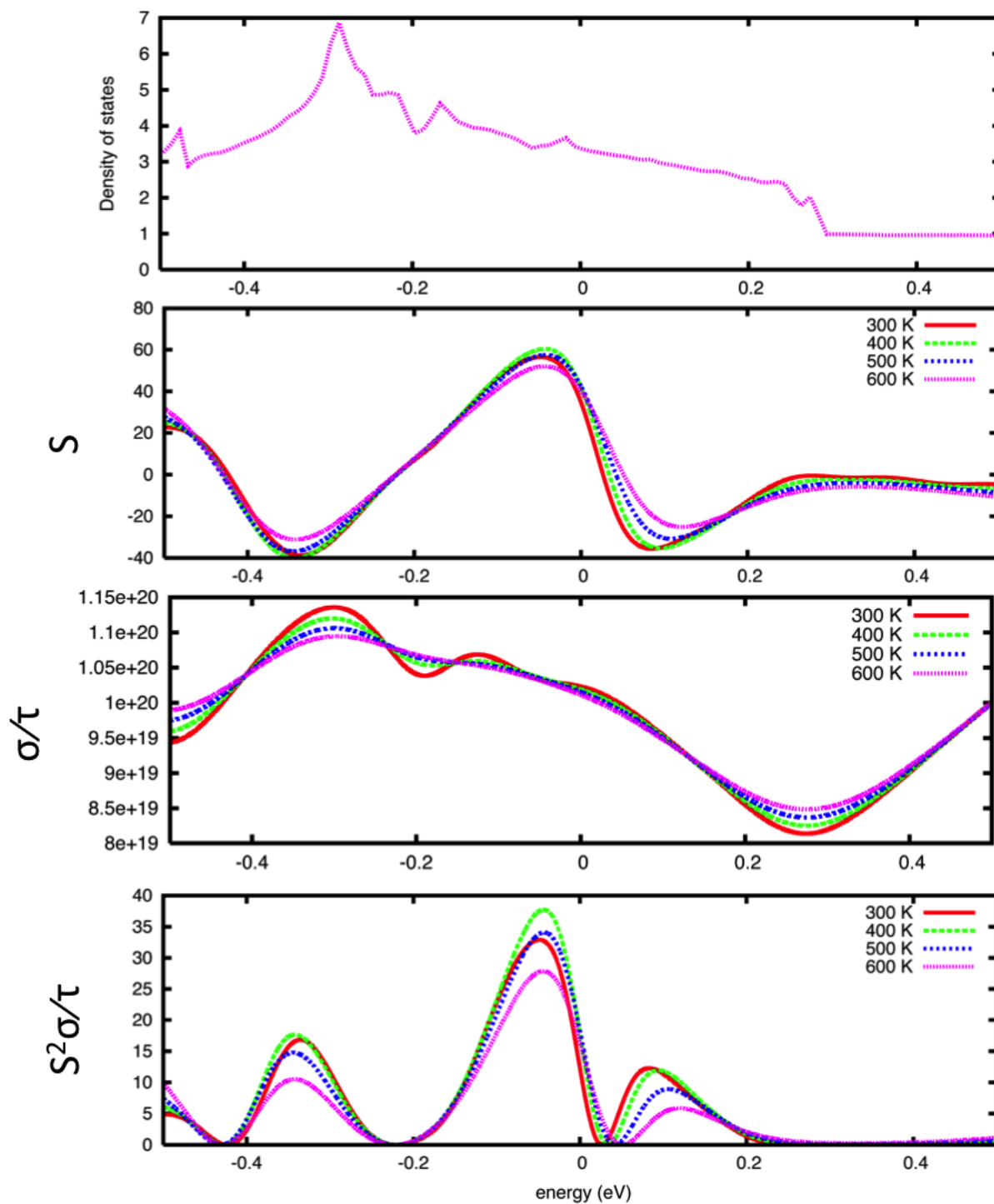
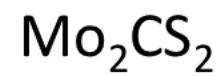


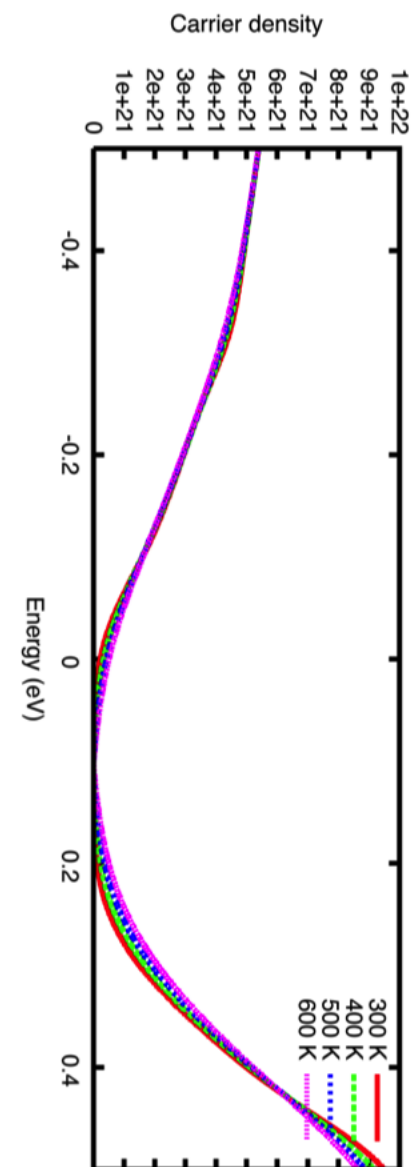
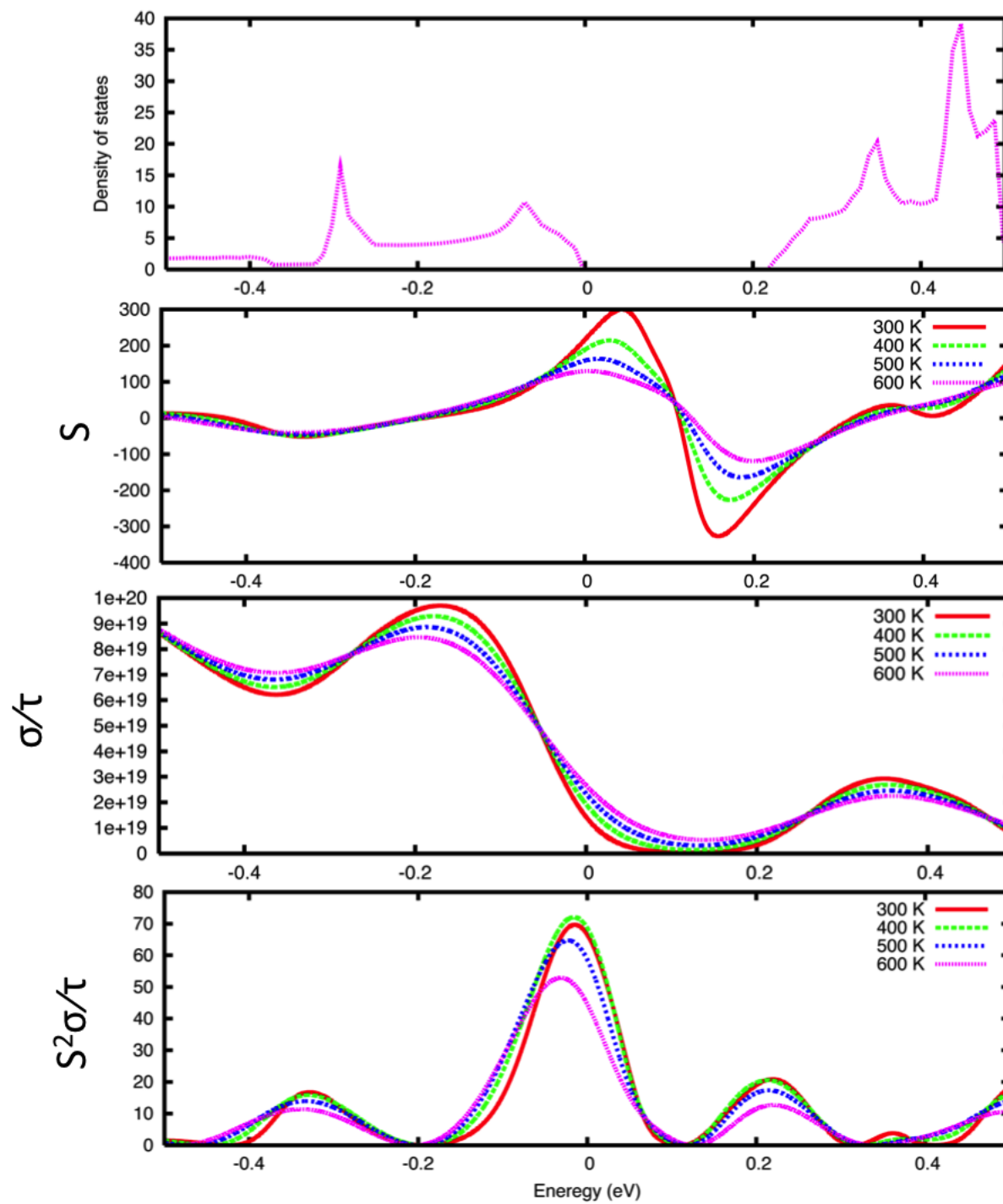
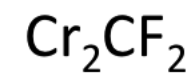
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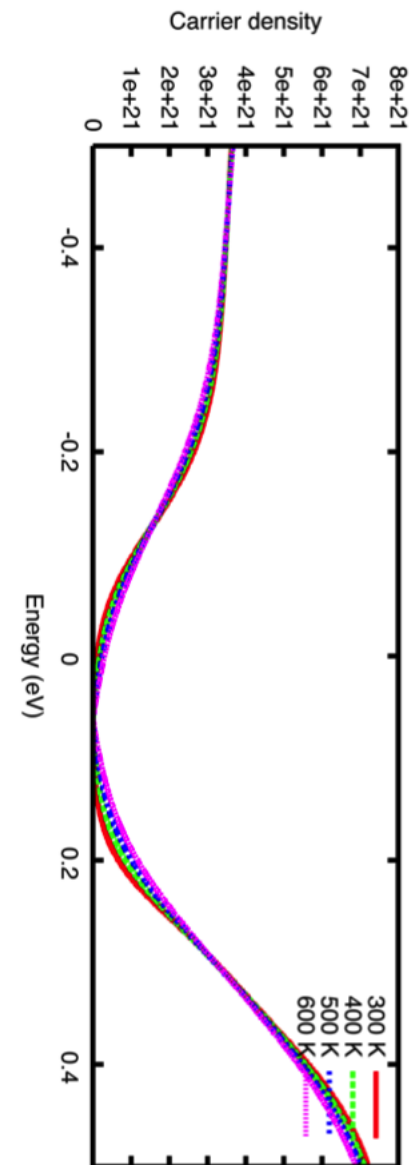
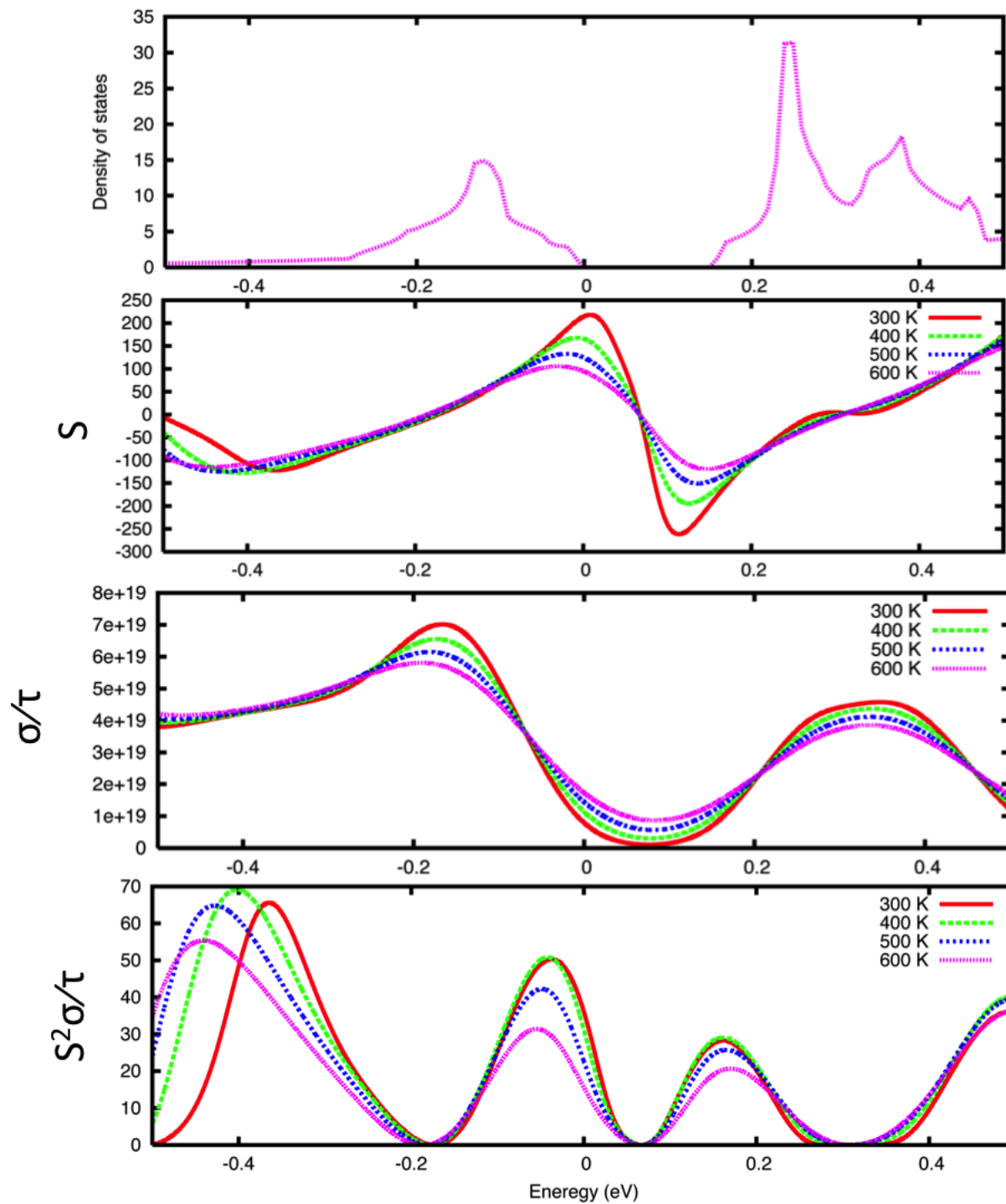
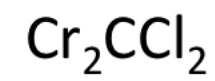


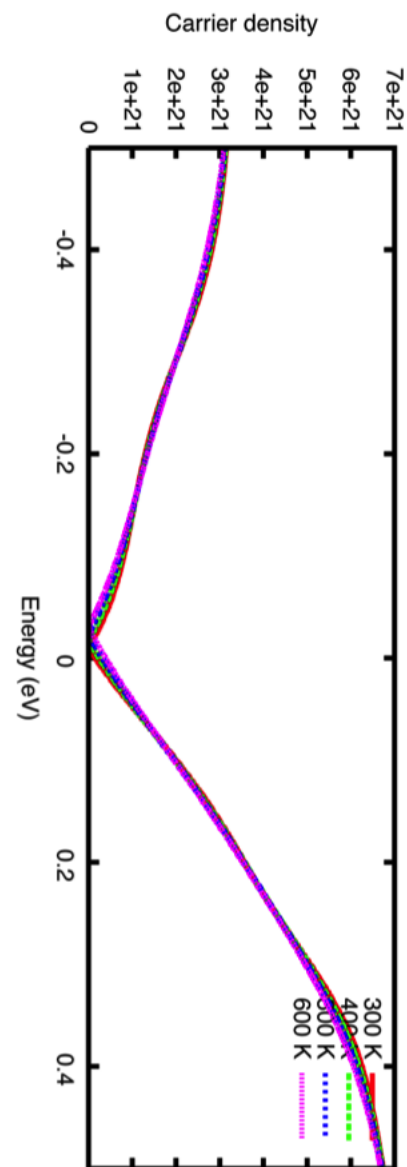
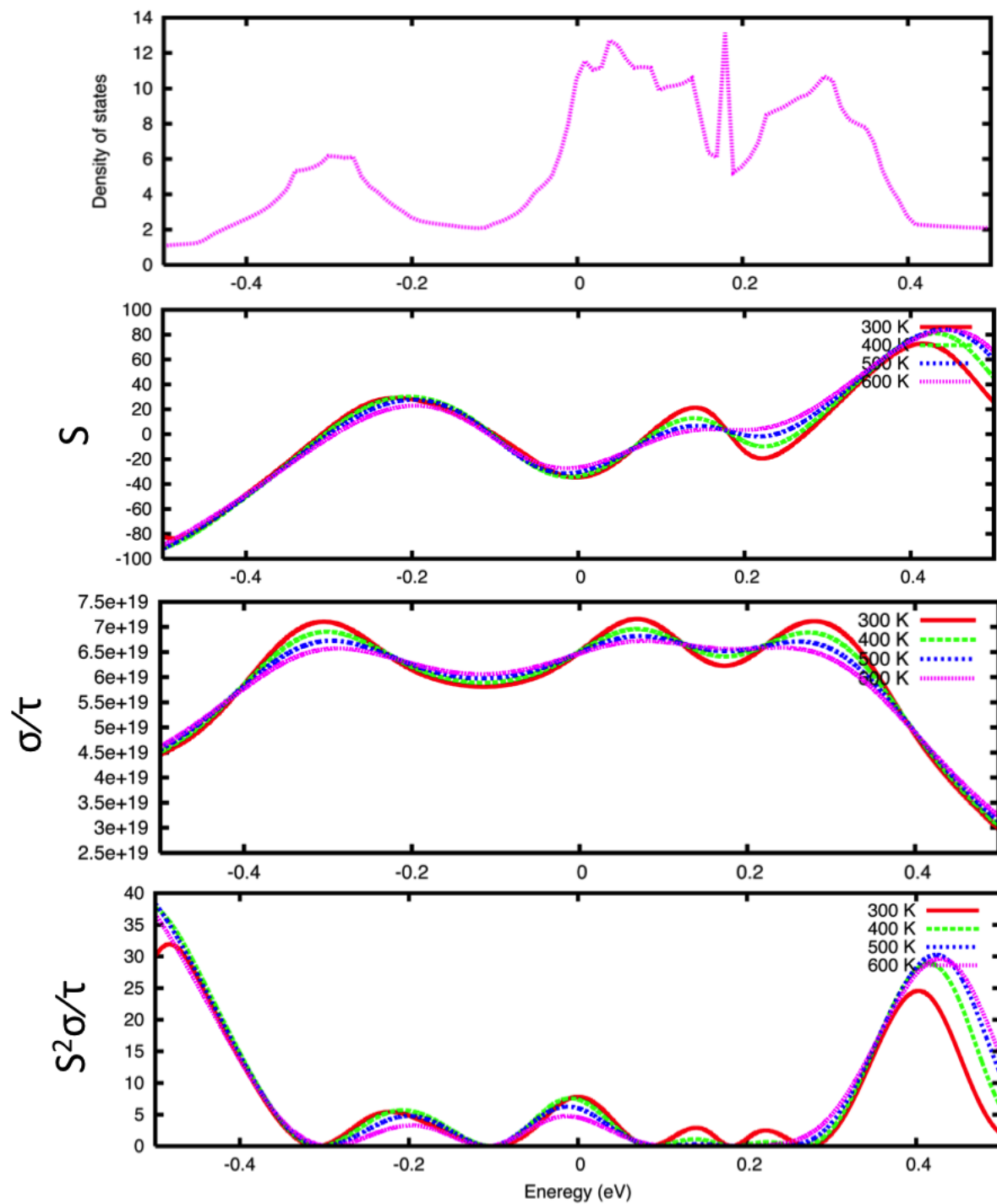
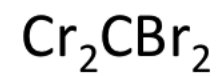


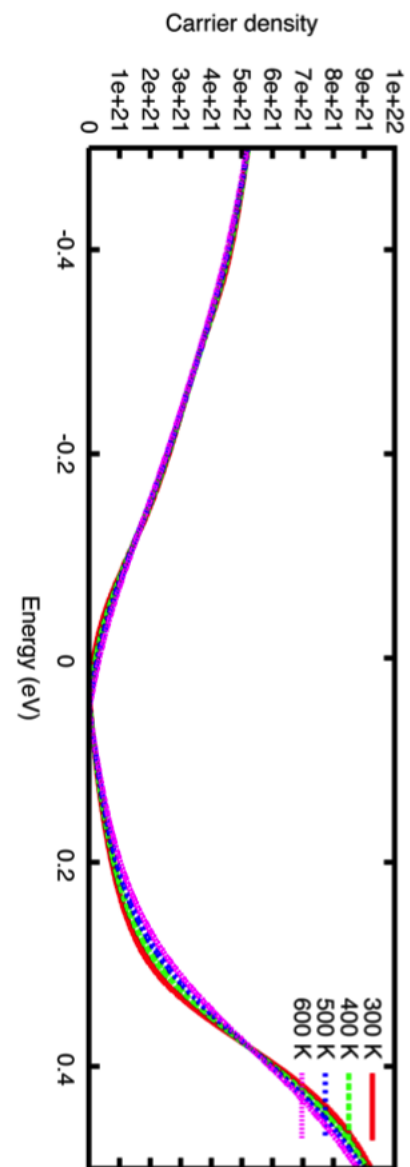
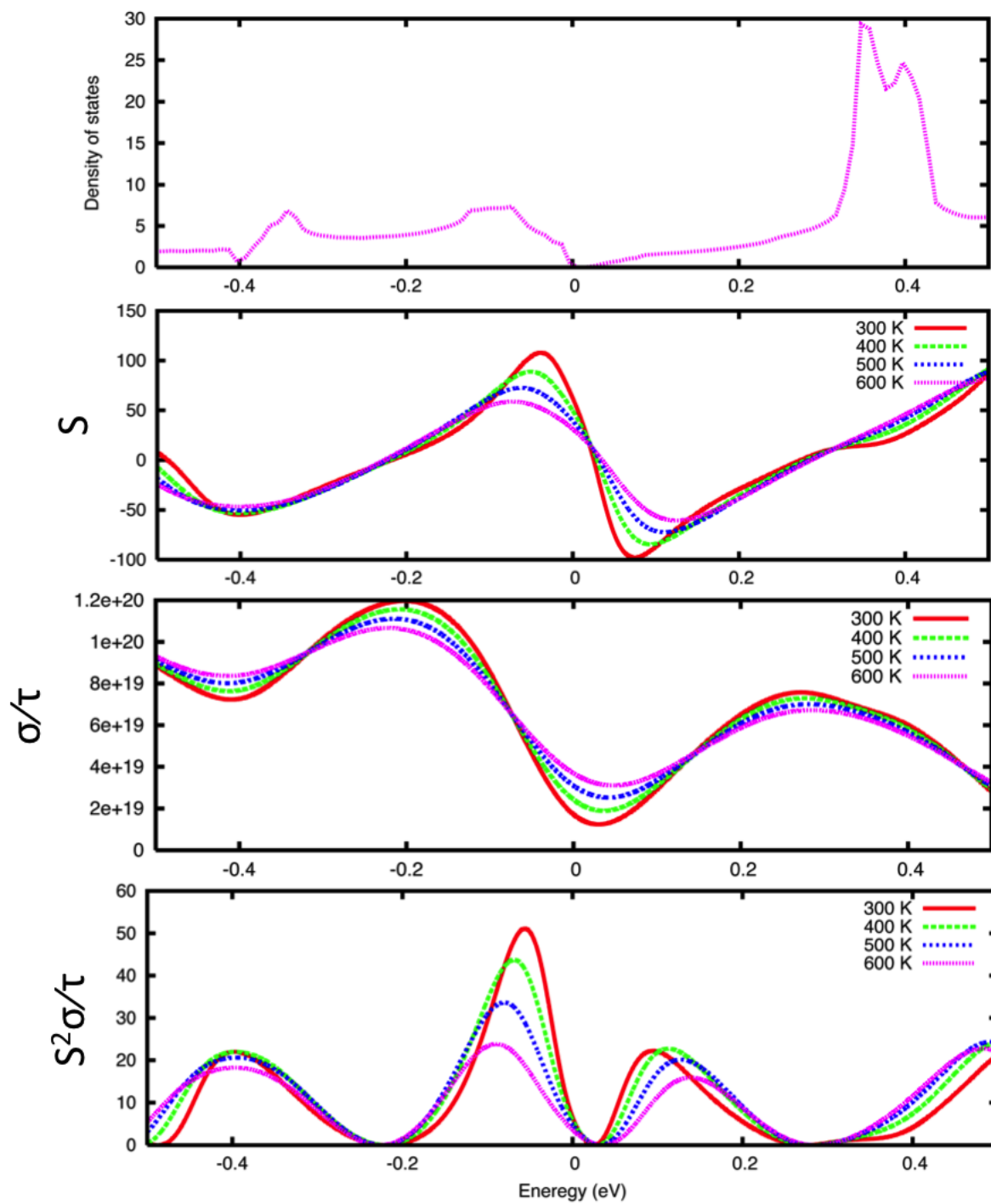
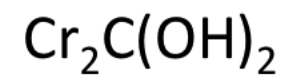


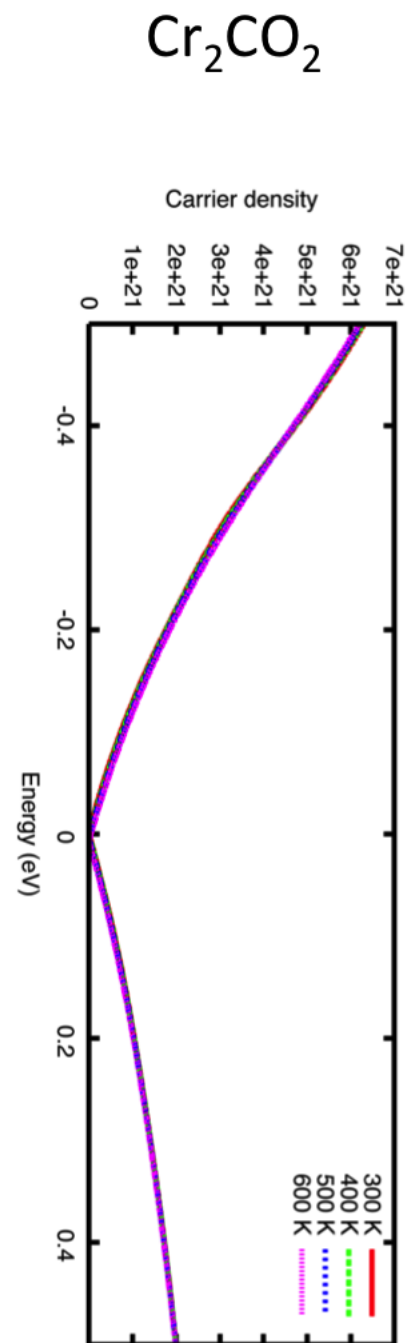
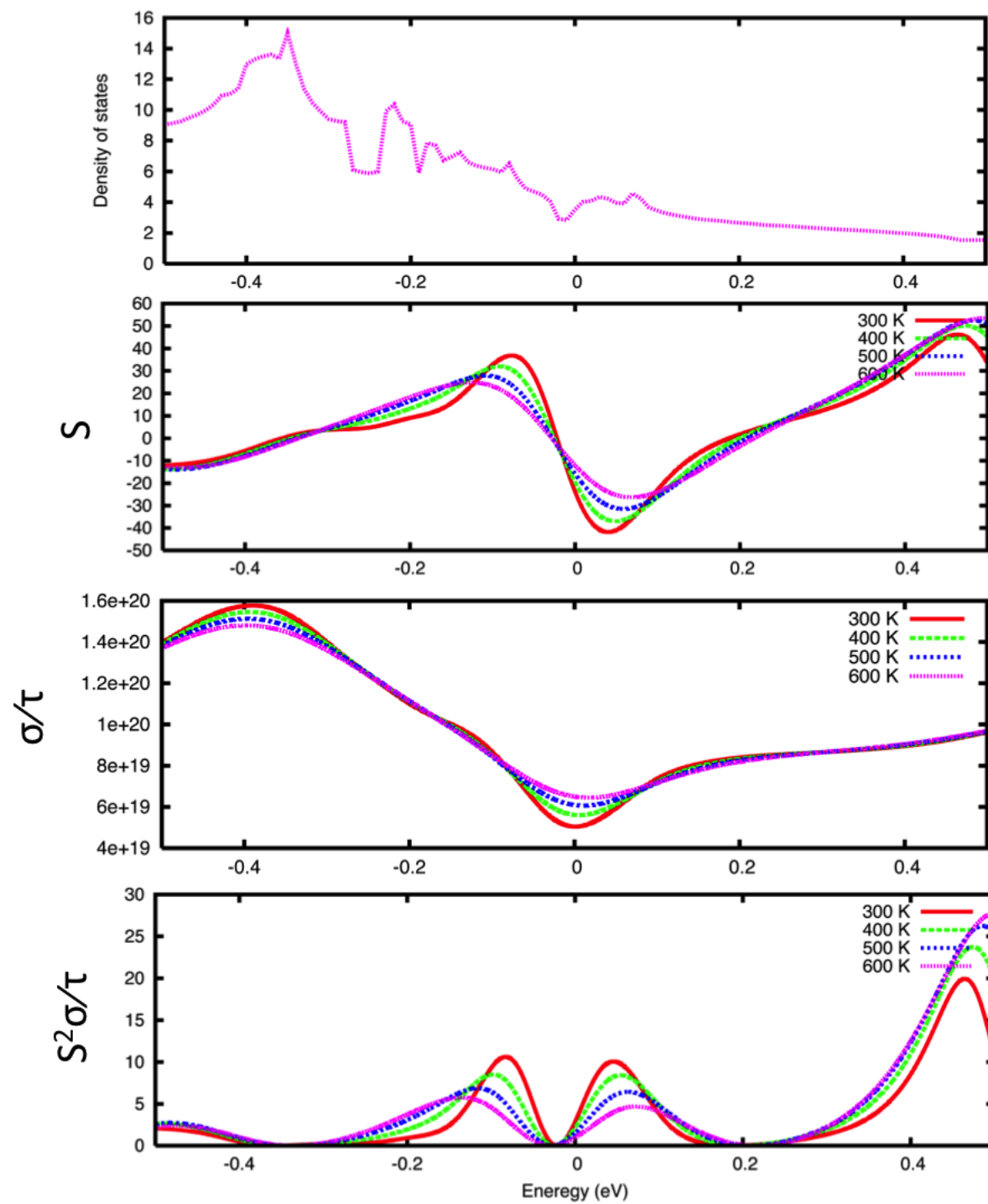


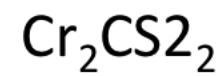




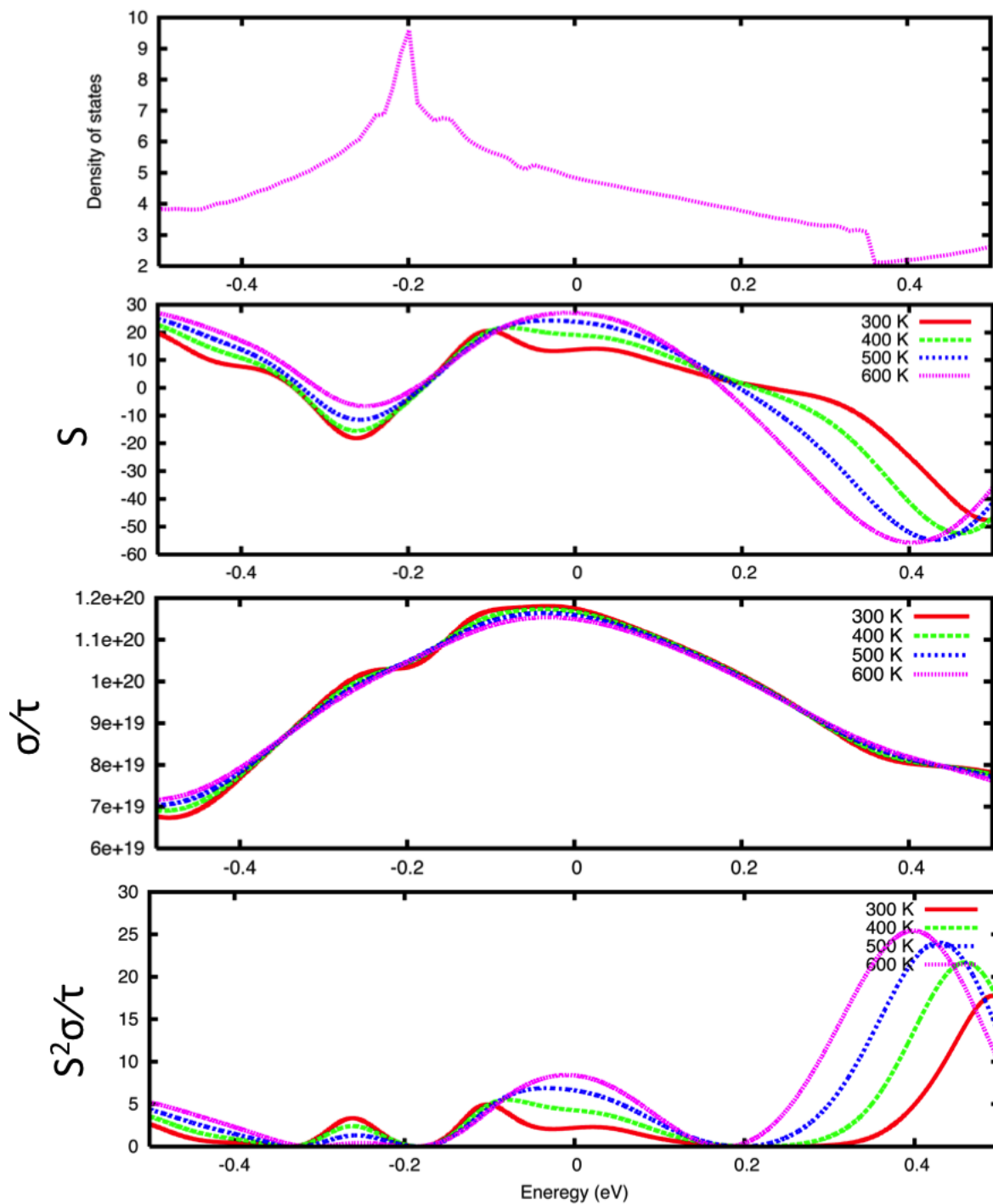
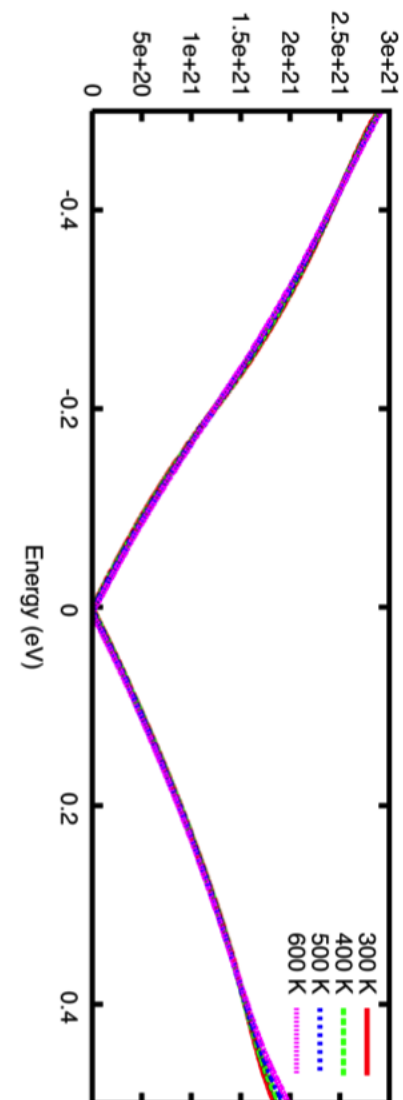








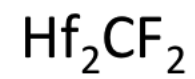
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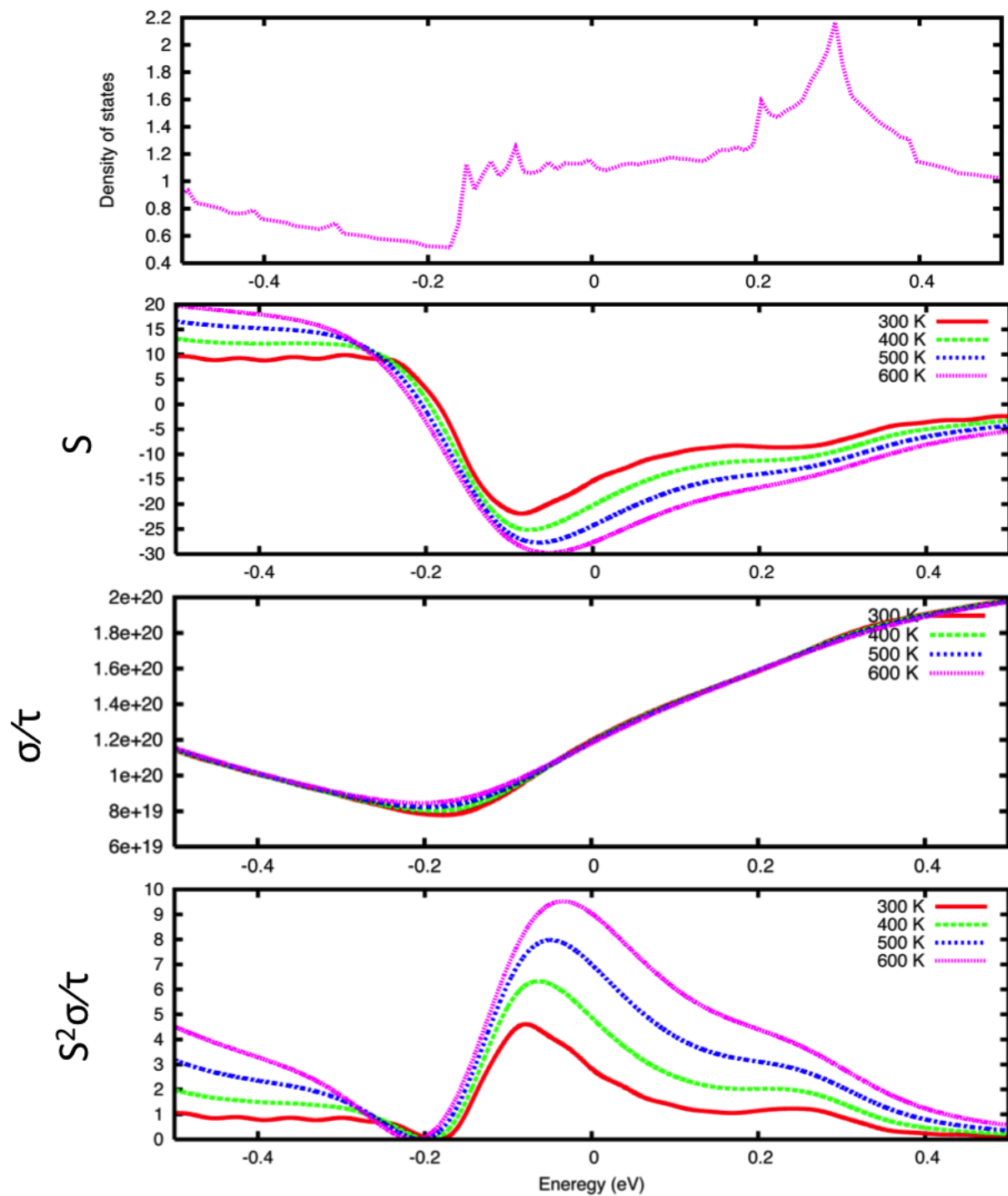
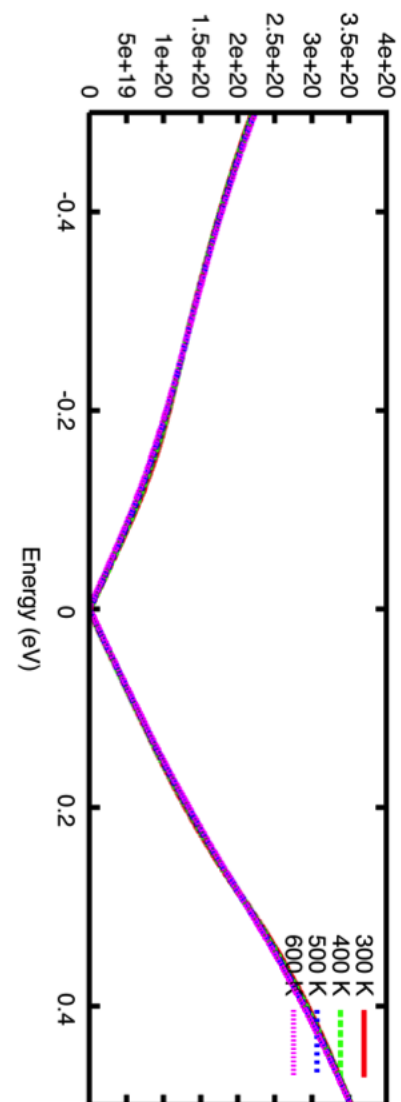
Thermoelectric properties of monolayer MXenes

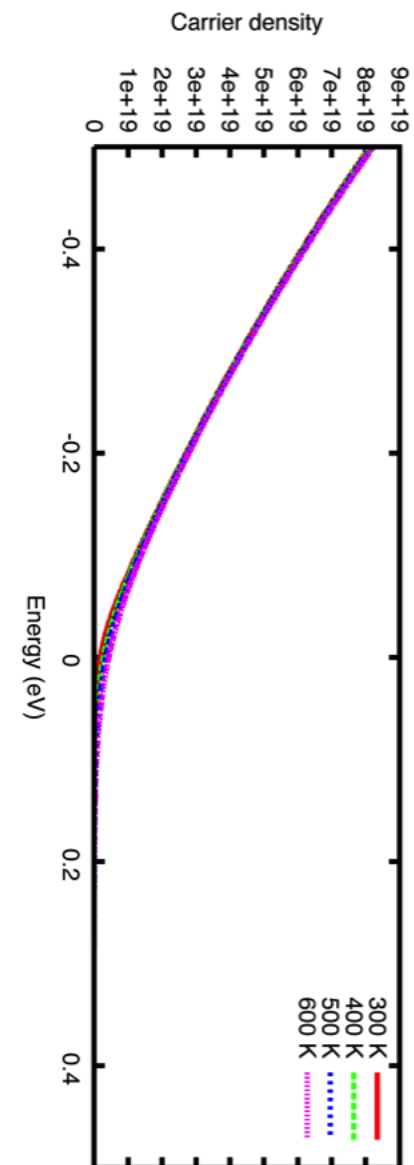
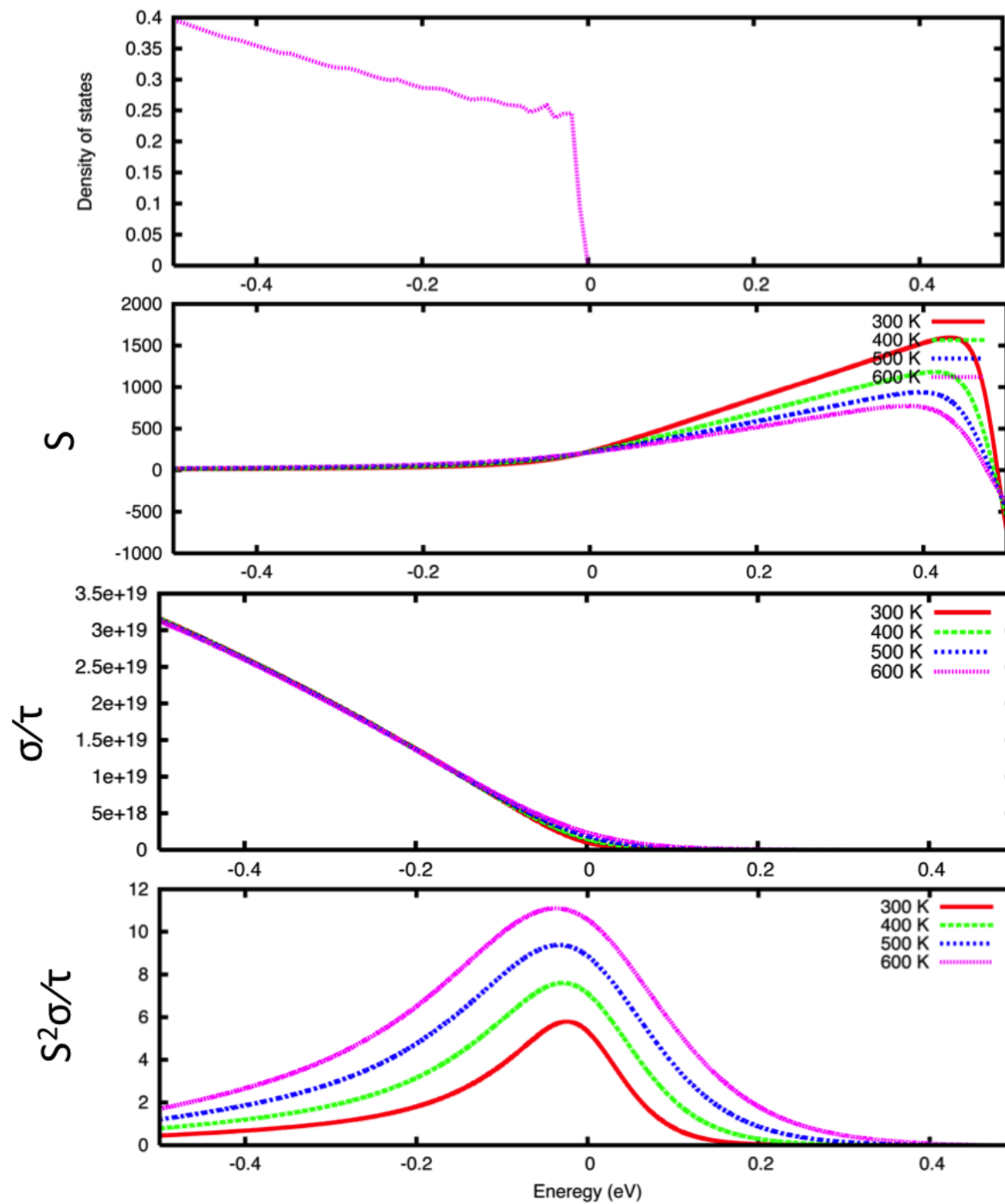
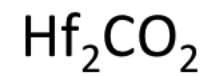
$$S = (S_{xx} + S_{yy})/2$$

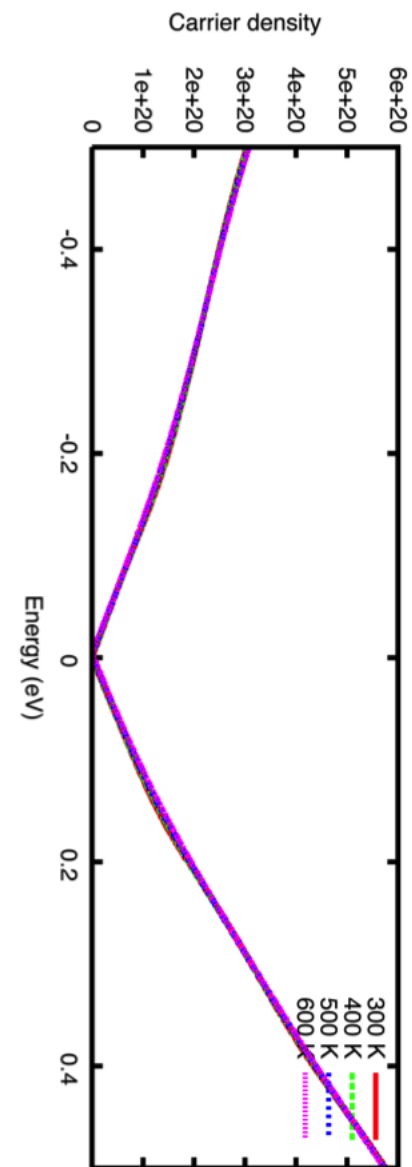
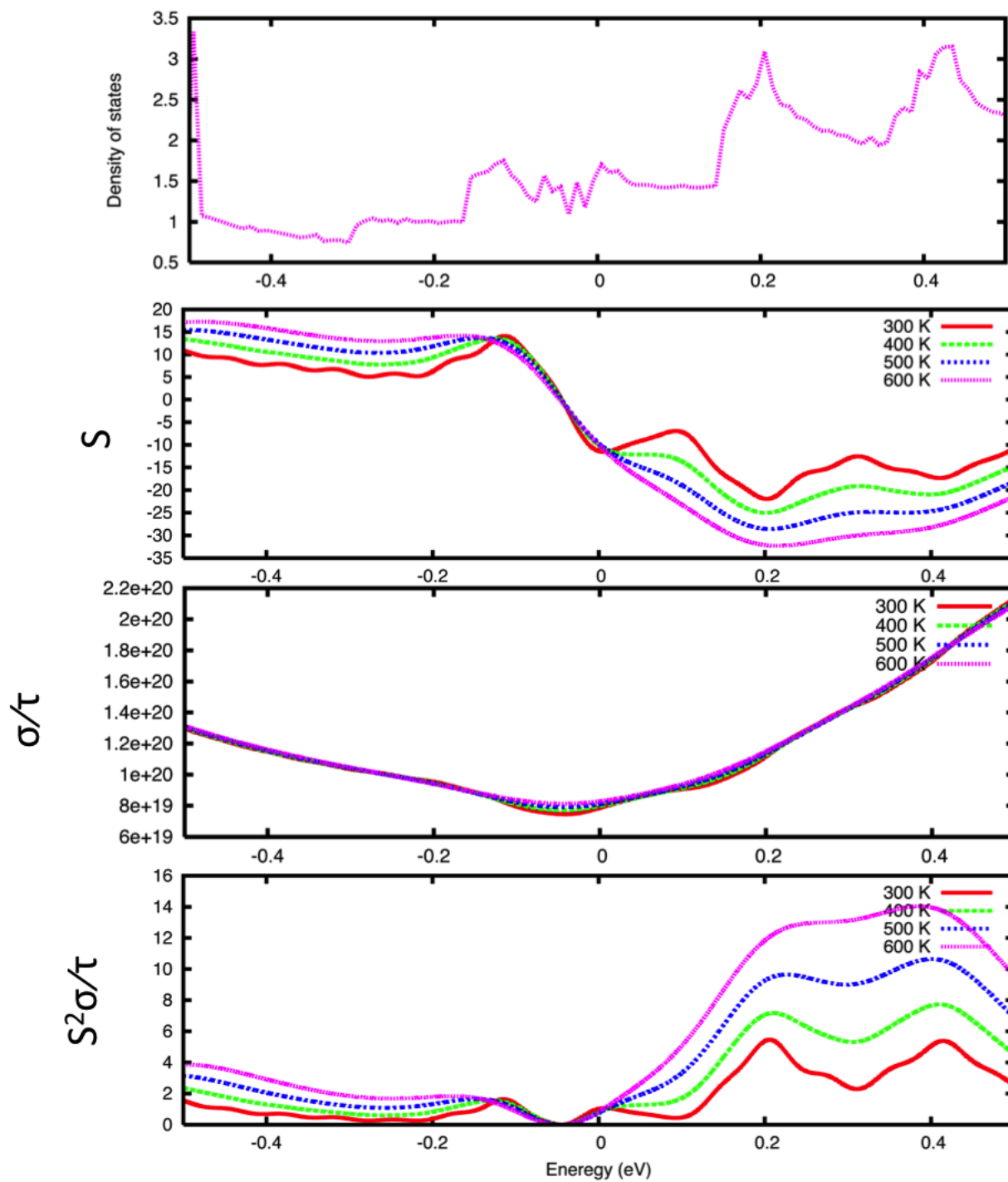
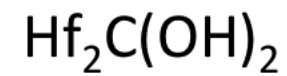
$$\sigma = (\sigma_{xx} + \sigma_{yy})/2$$

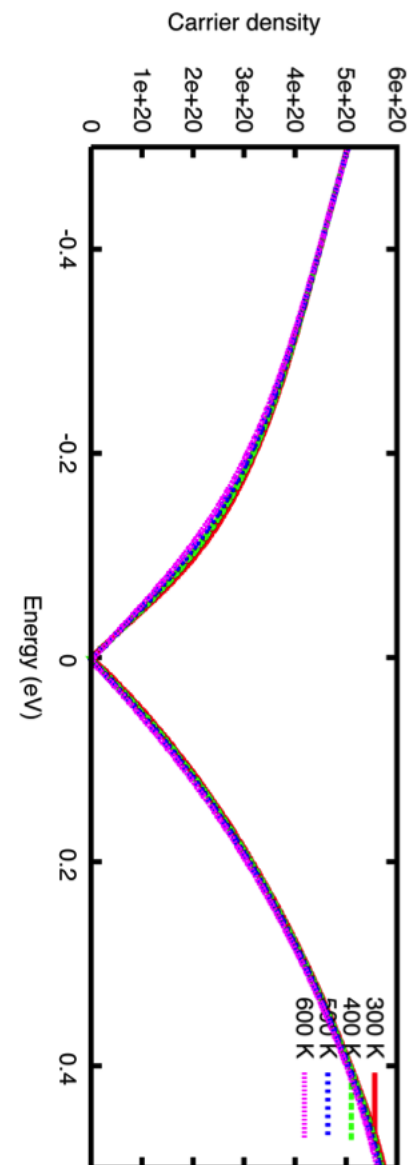
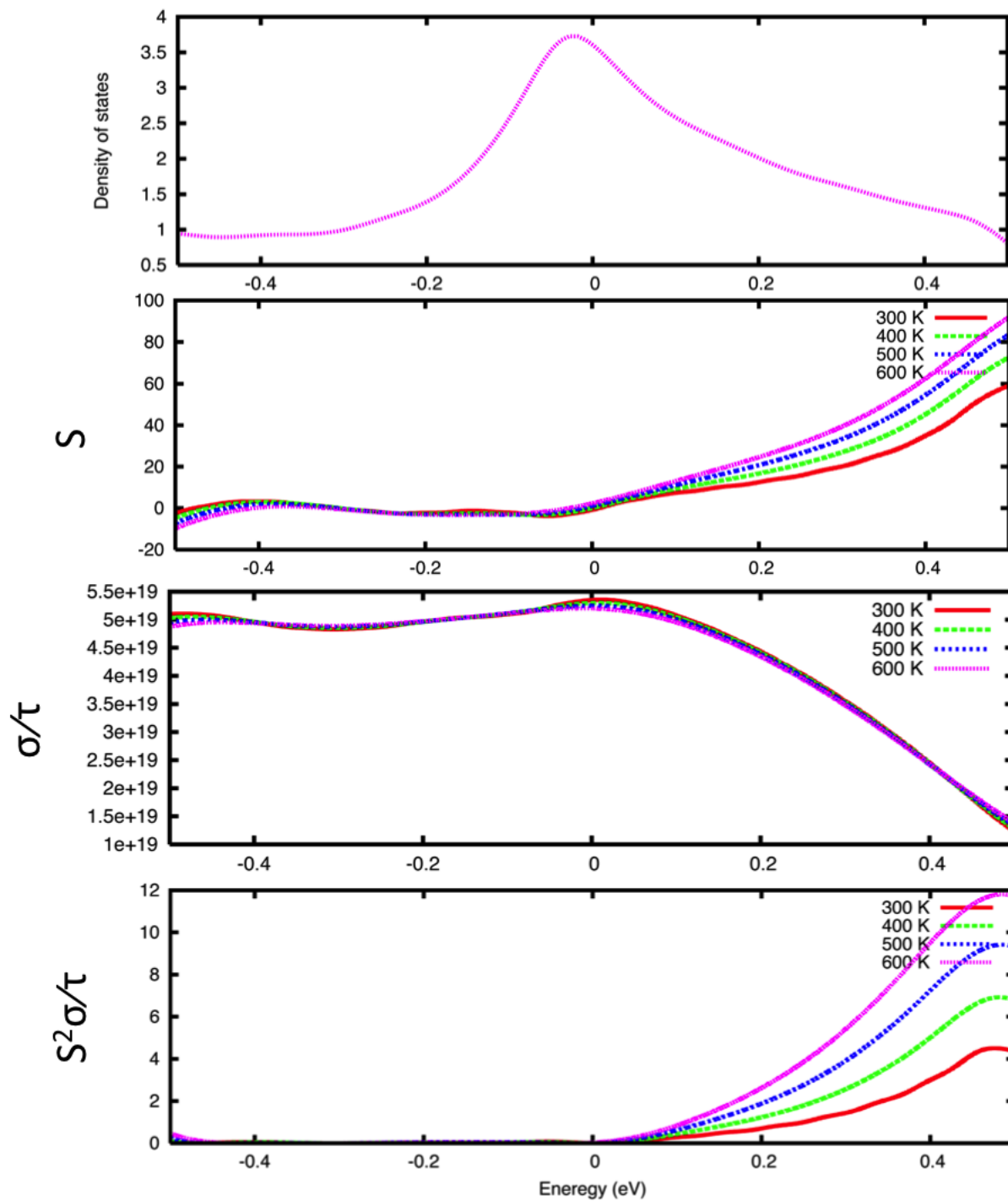
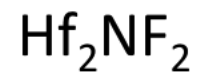


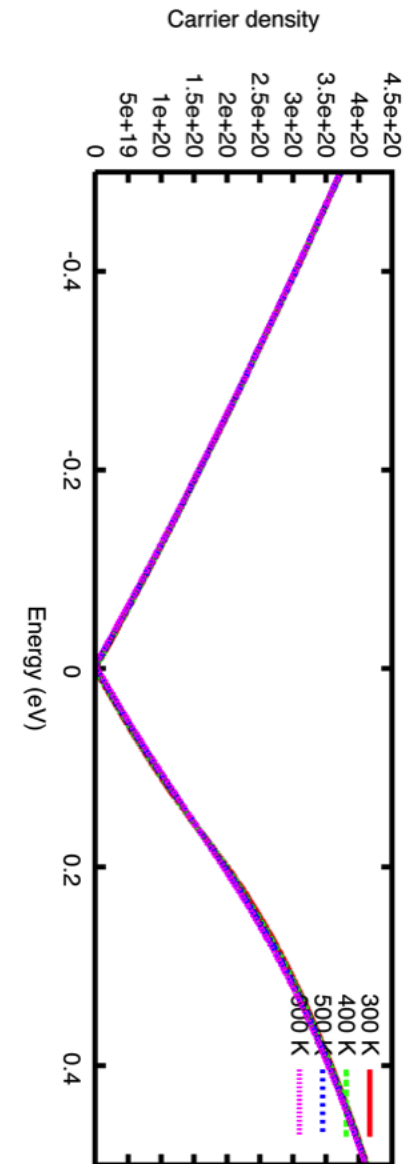
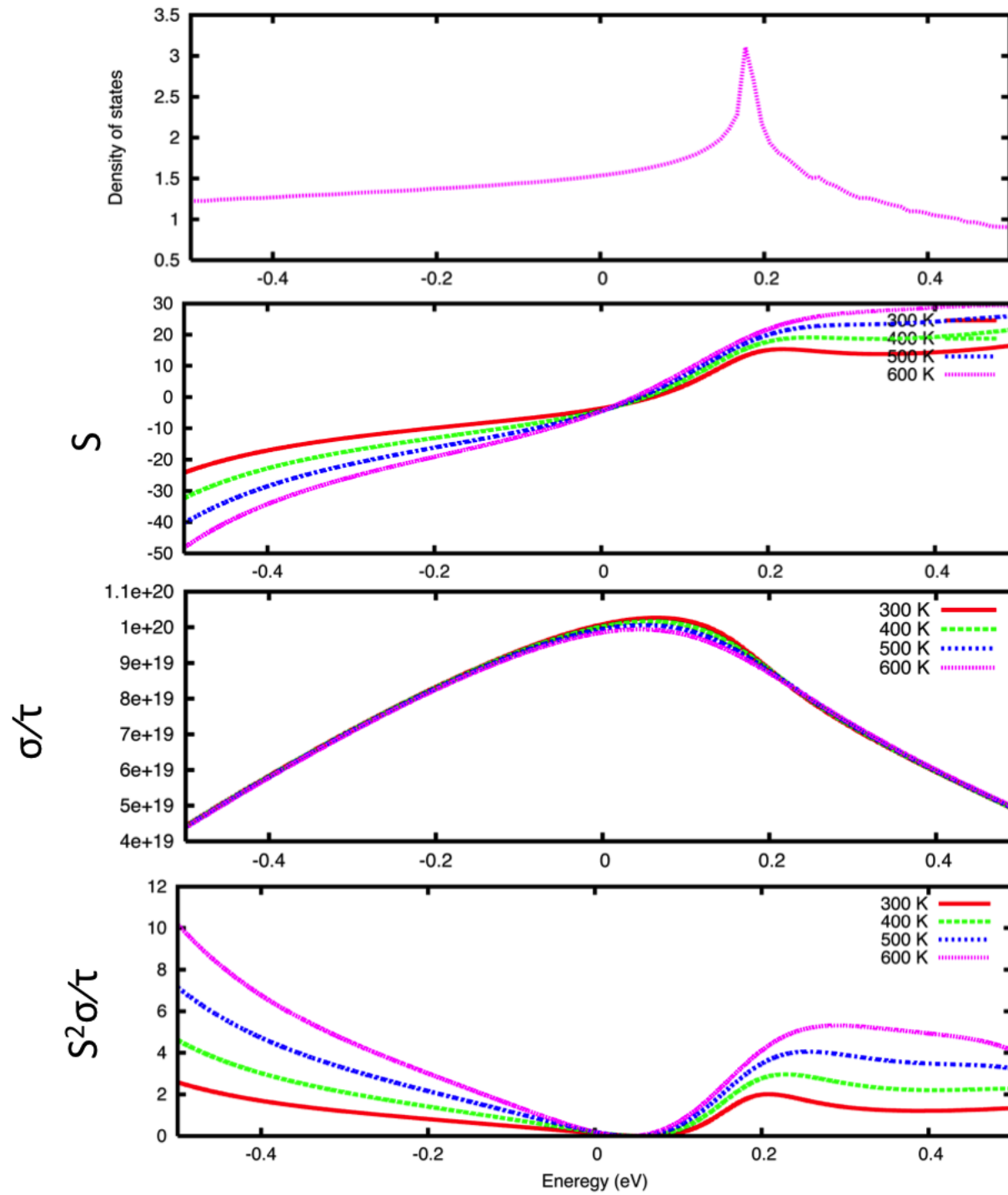
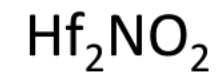
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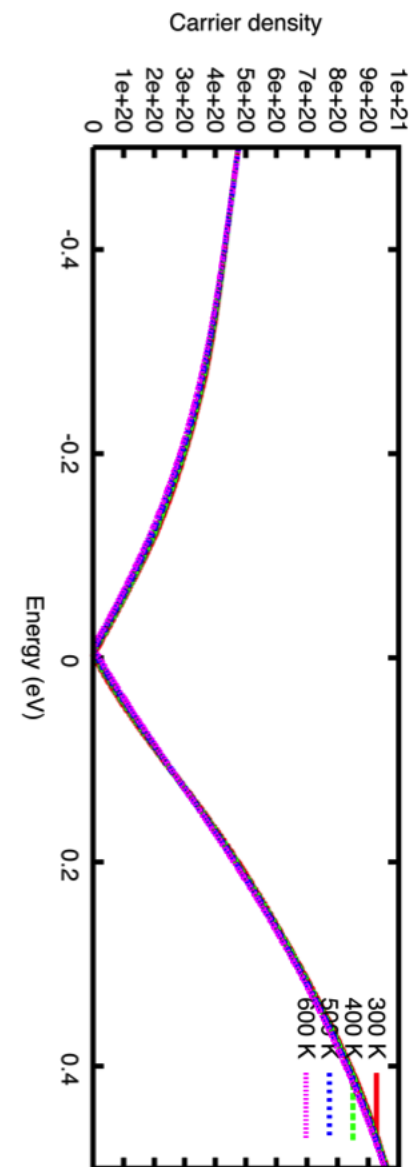
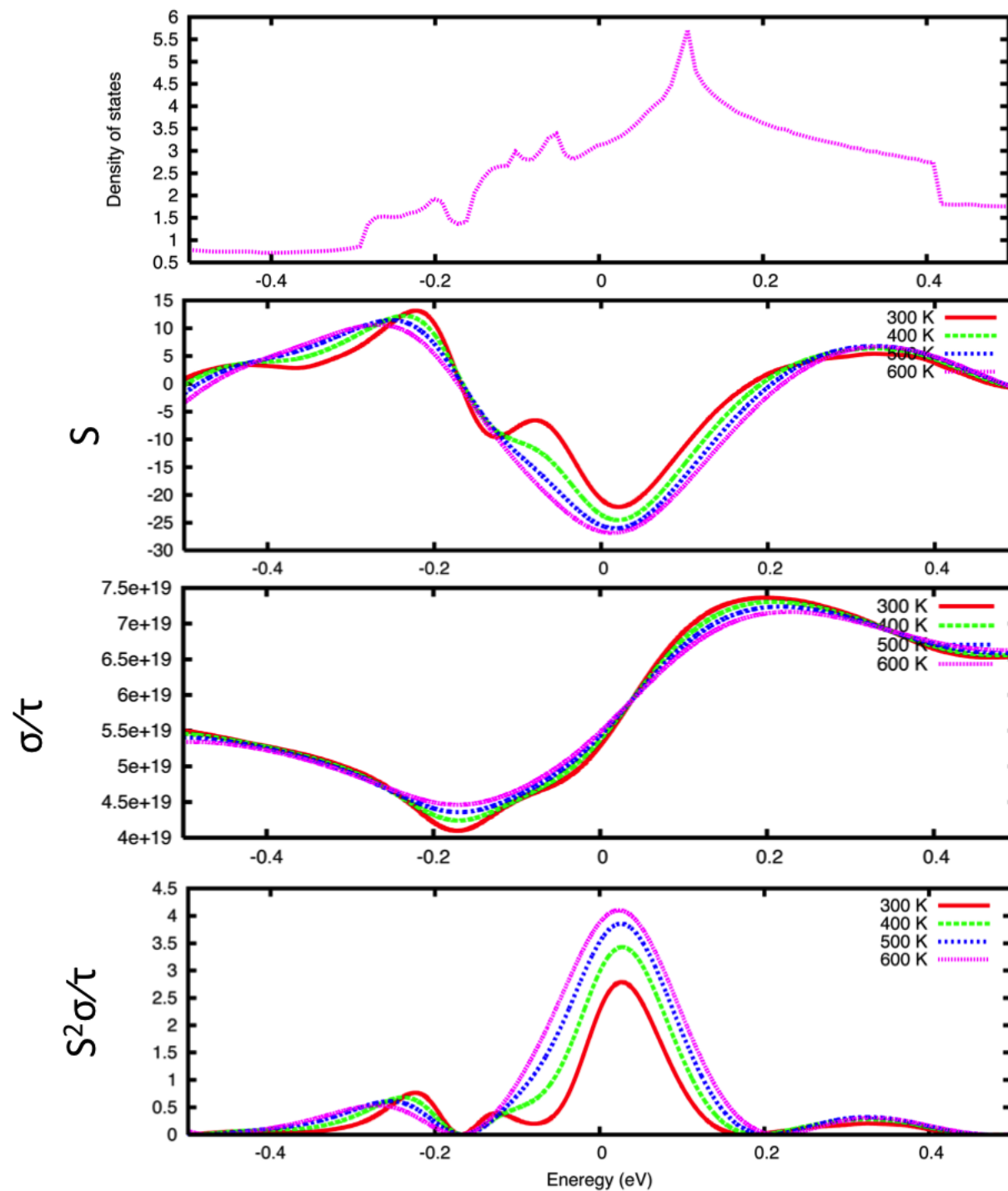
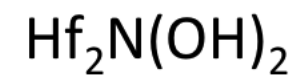


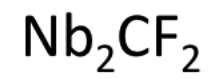




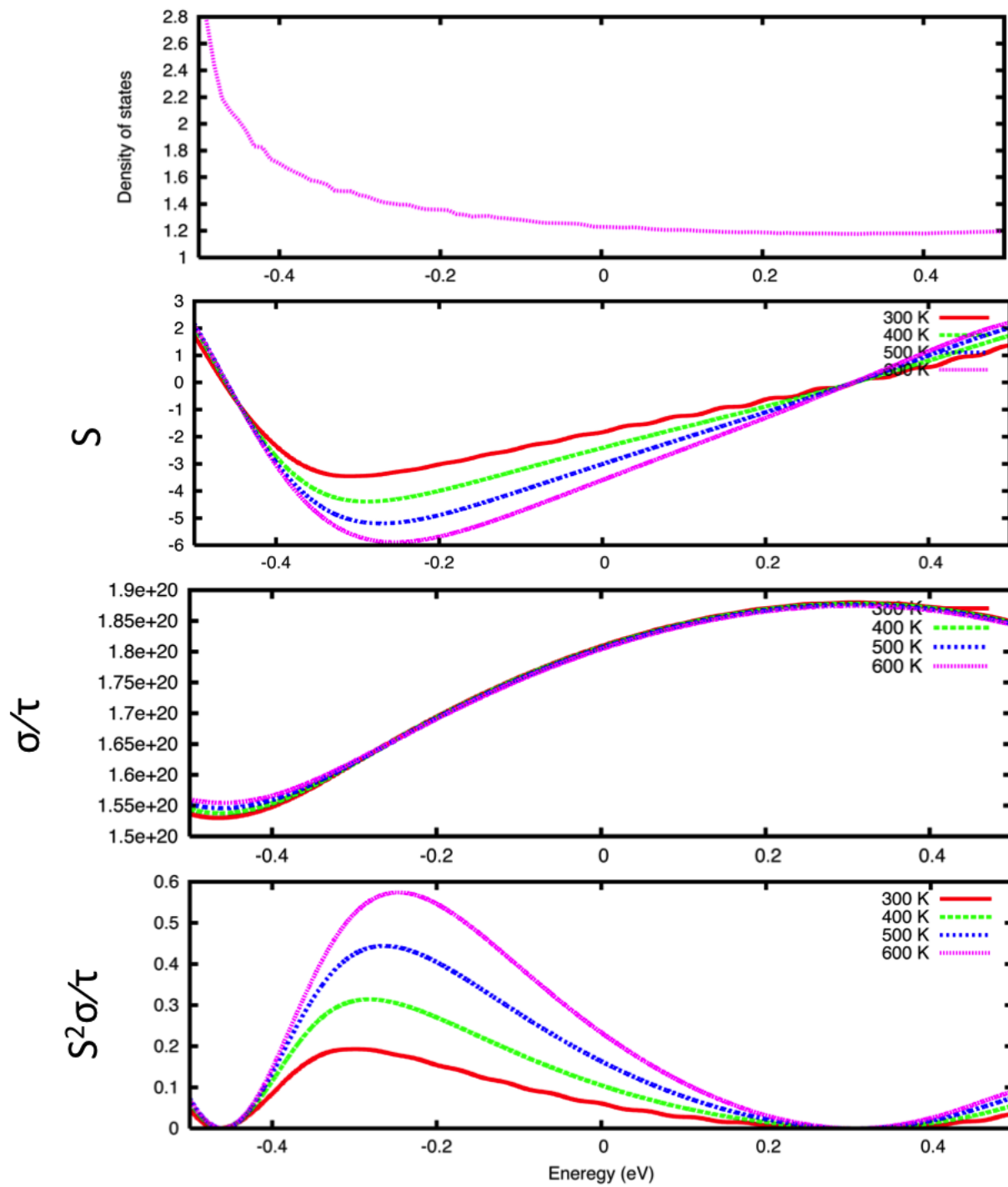
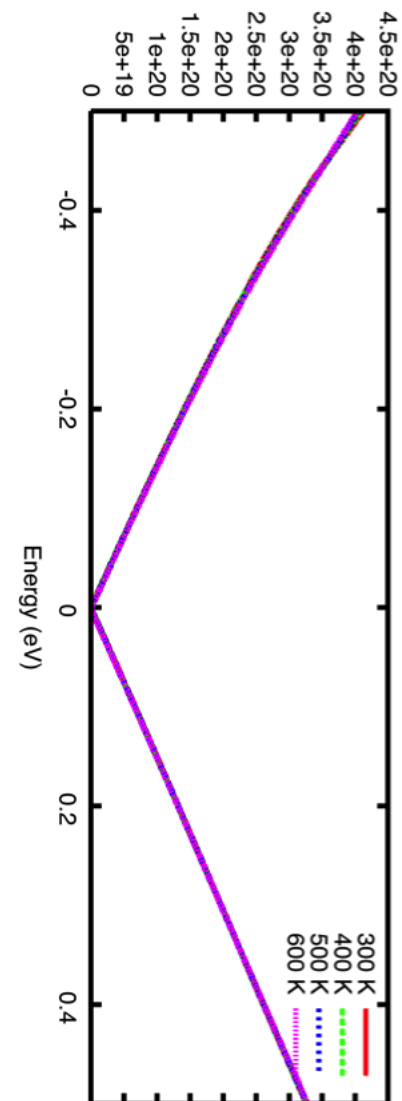


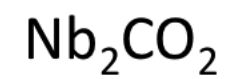




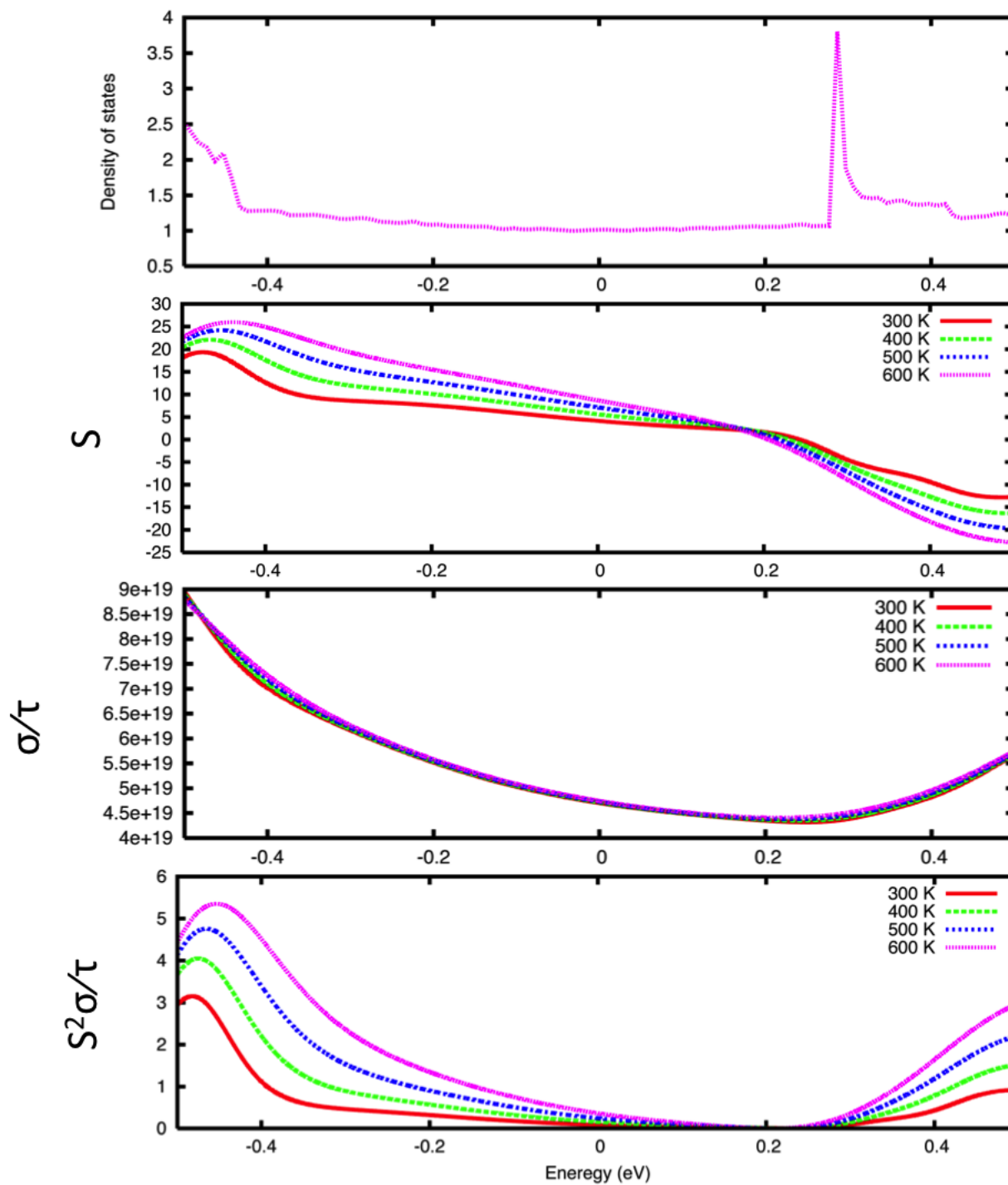
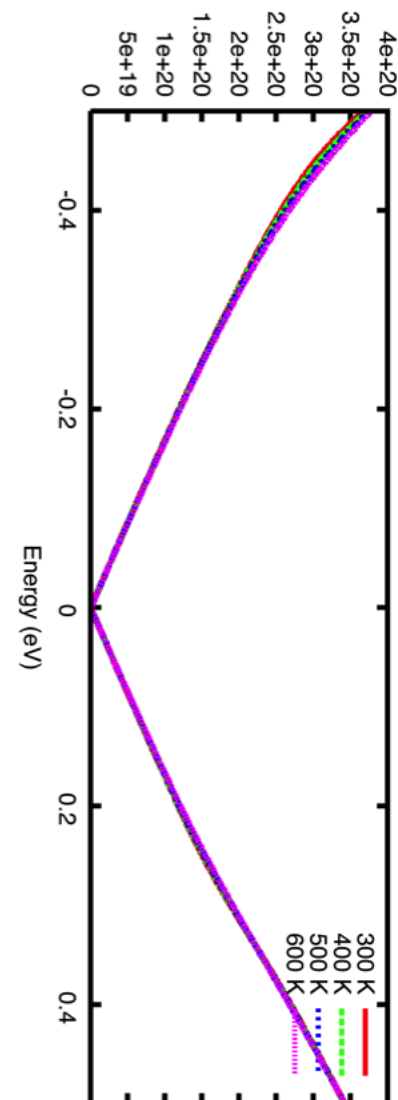


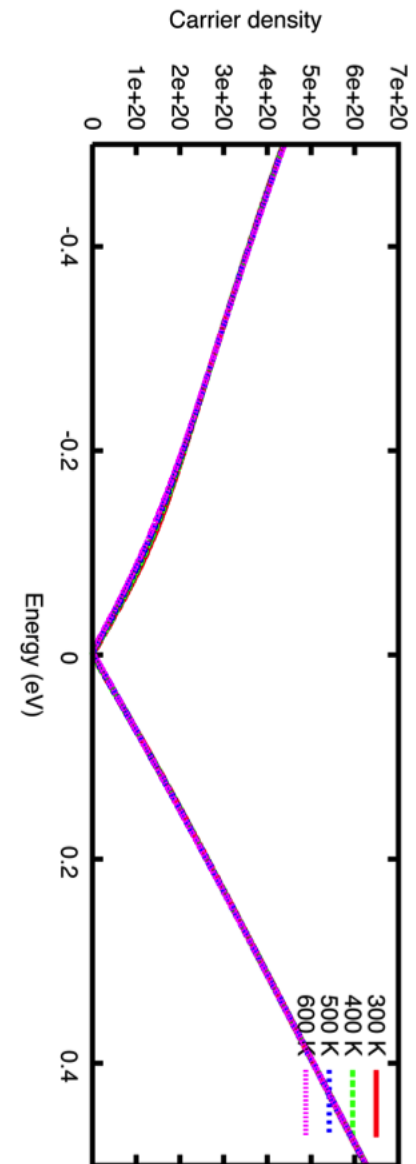
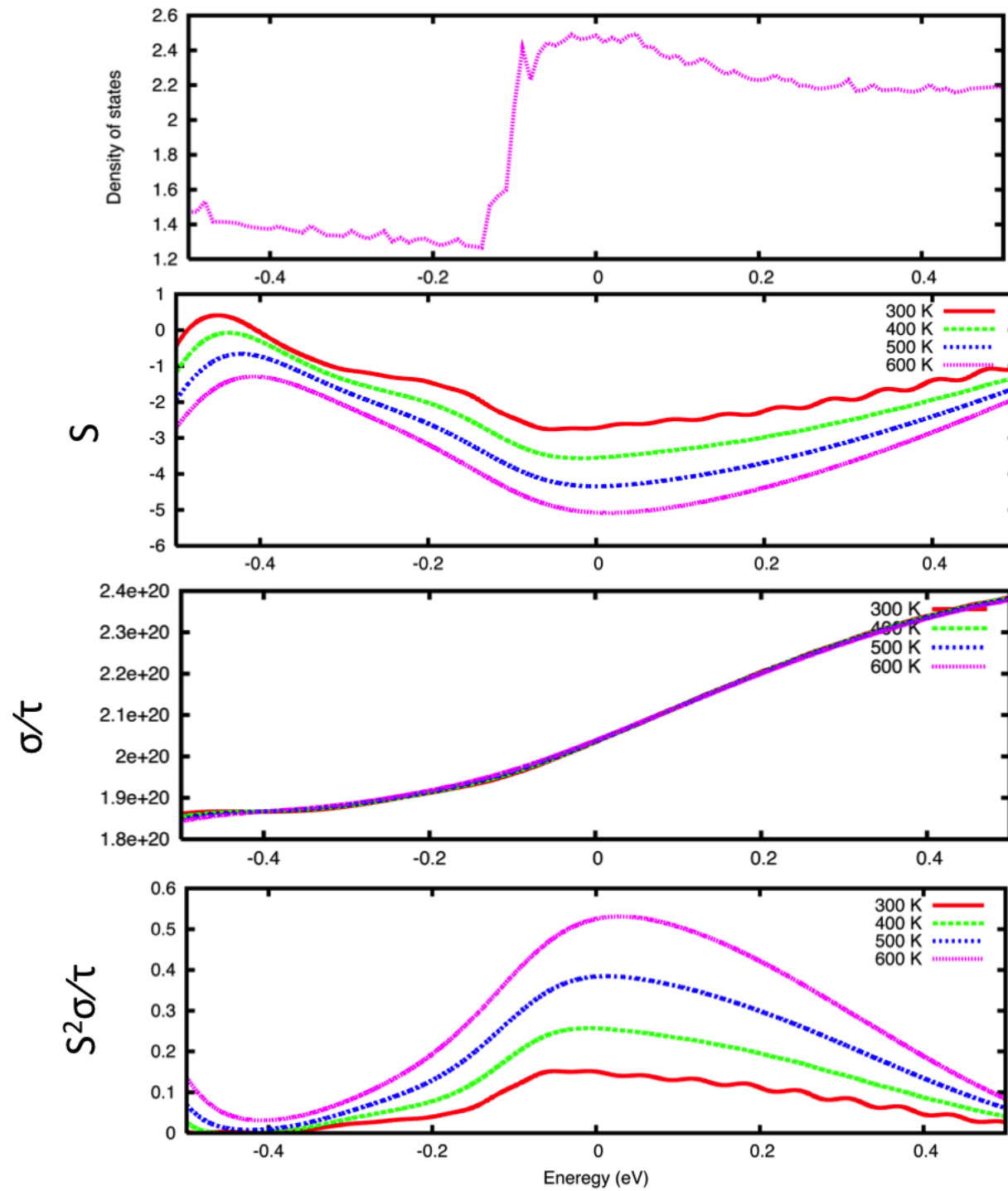
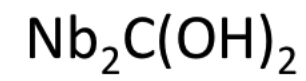
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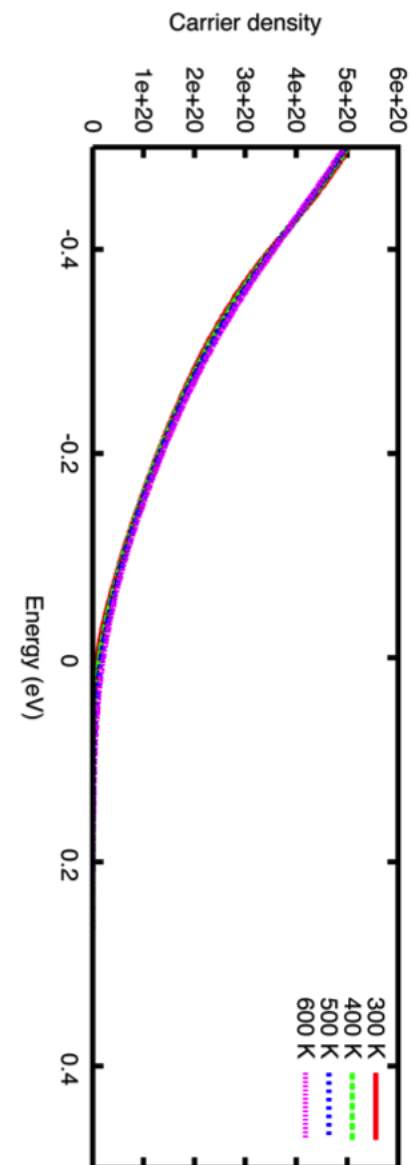
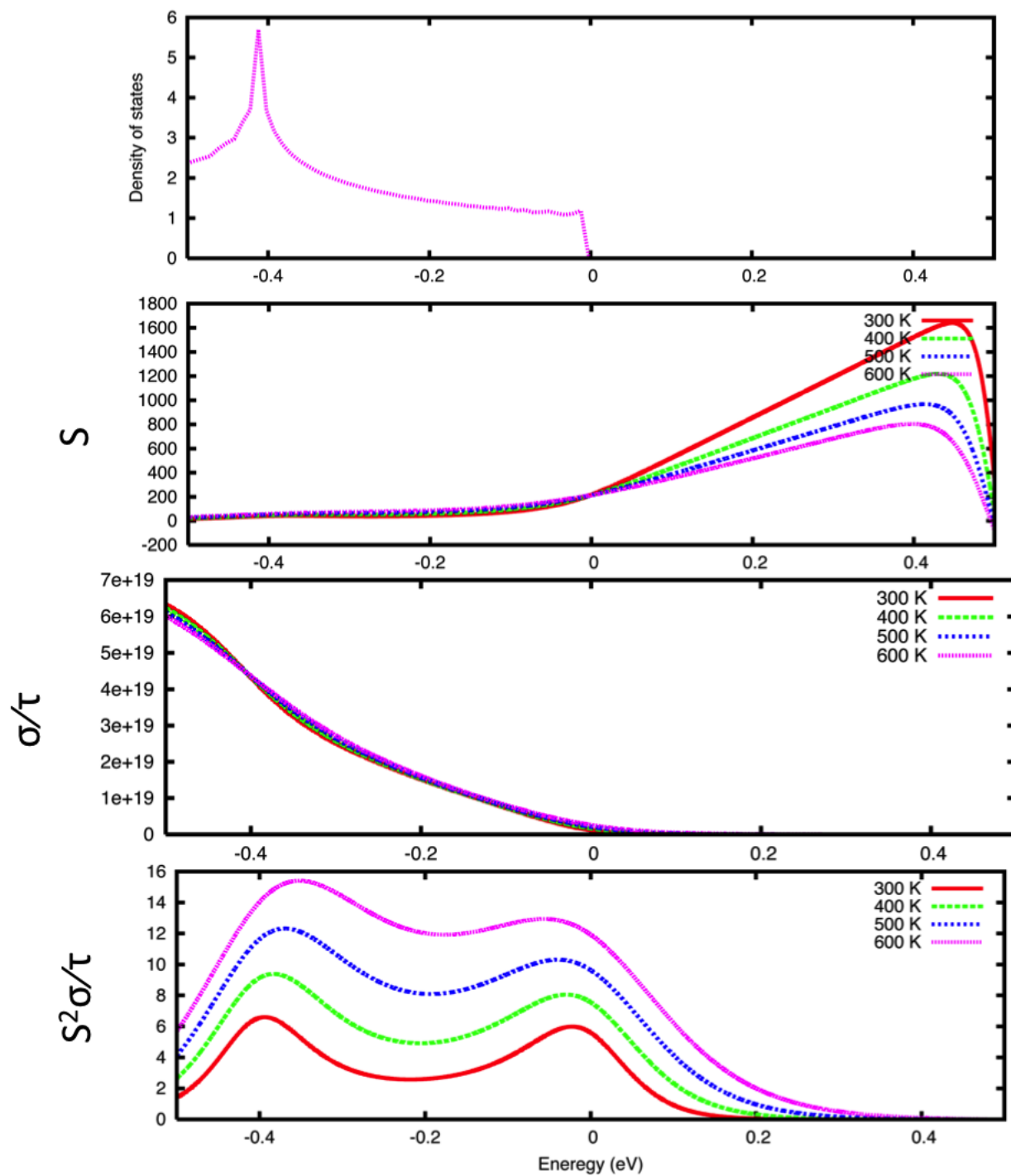
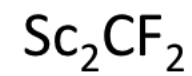


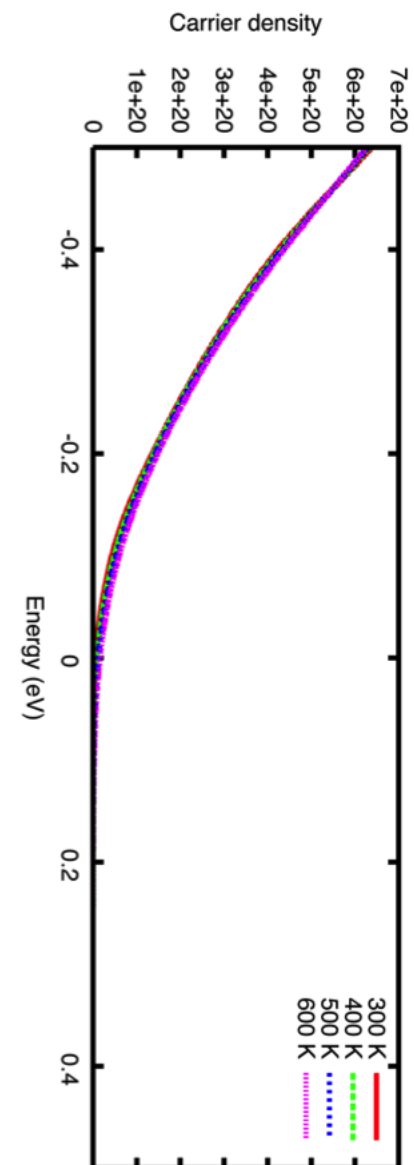
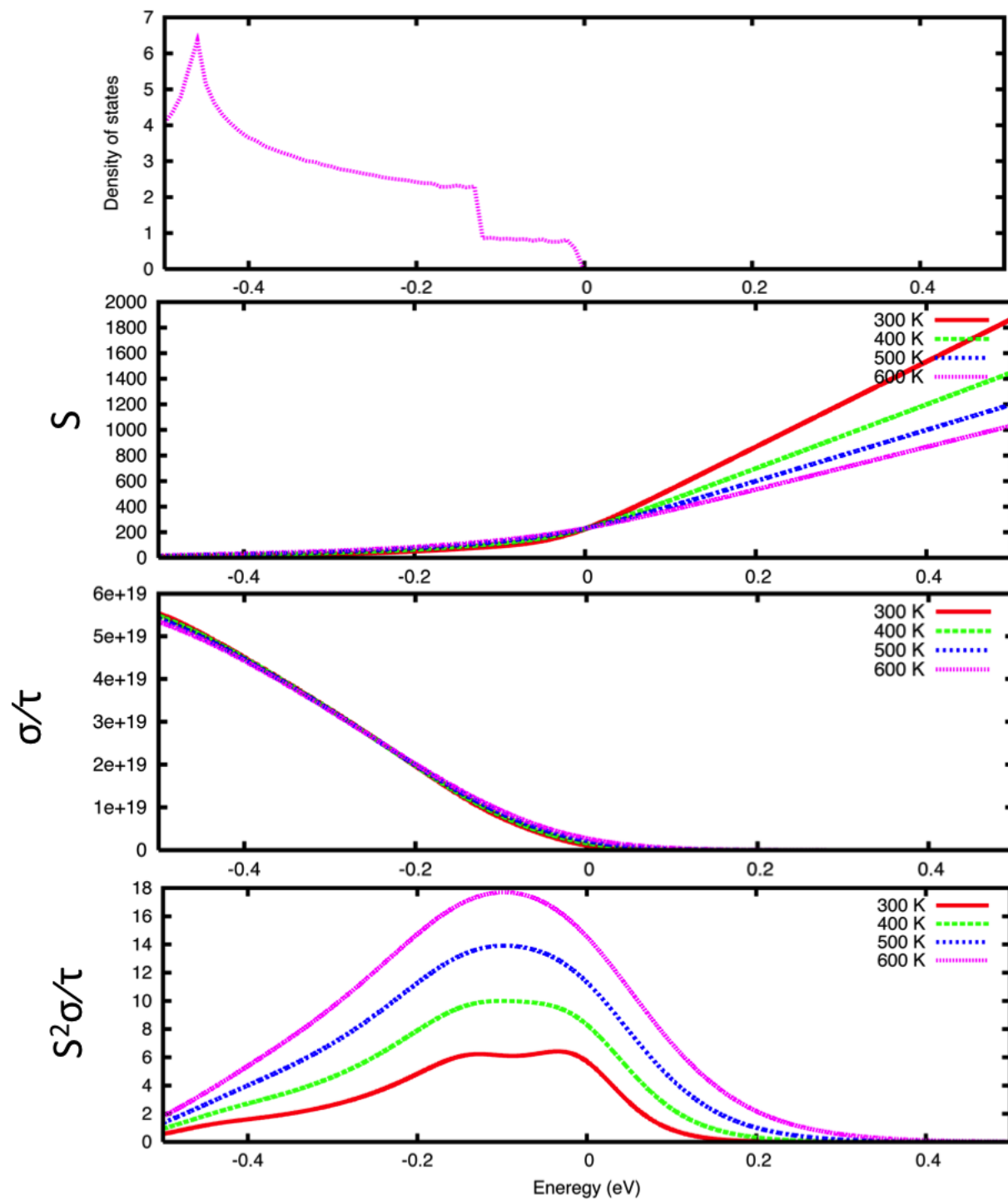
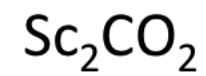


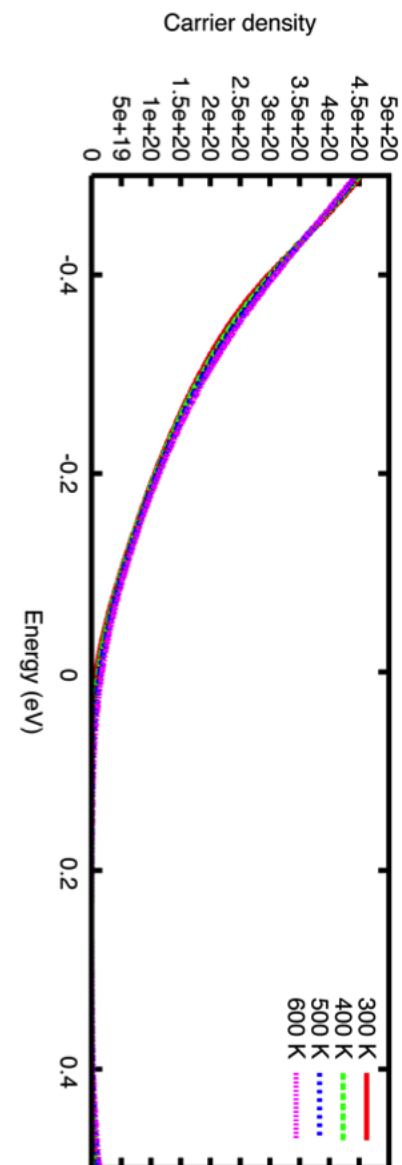
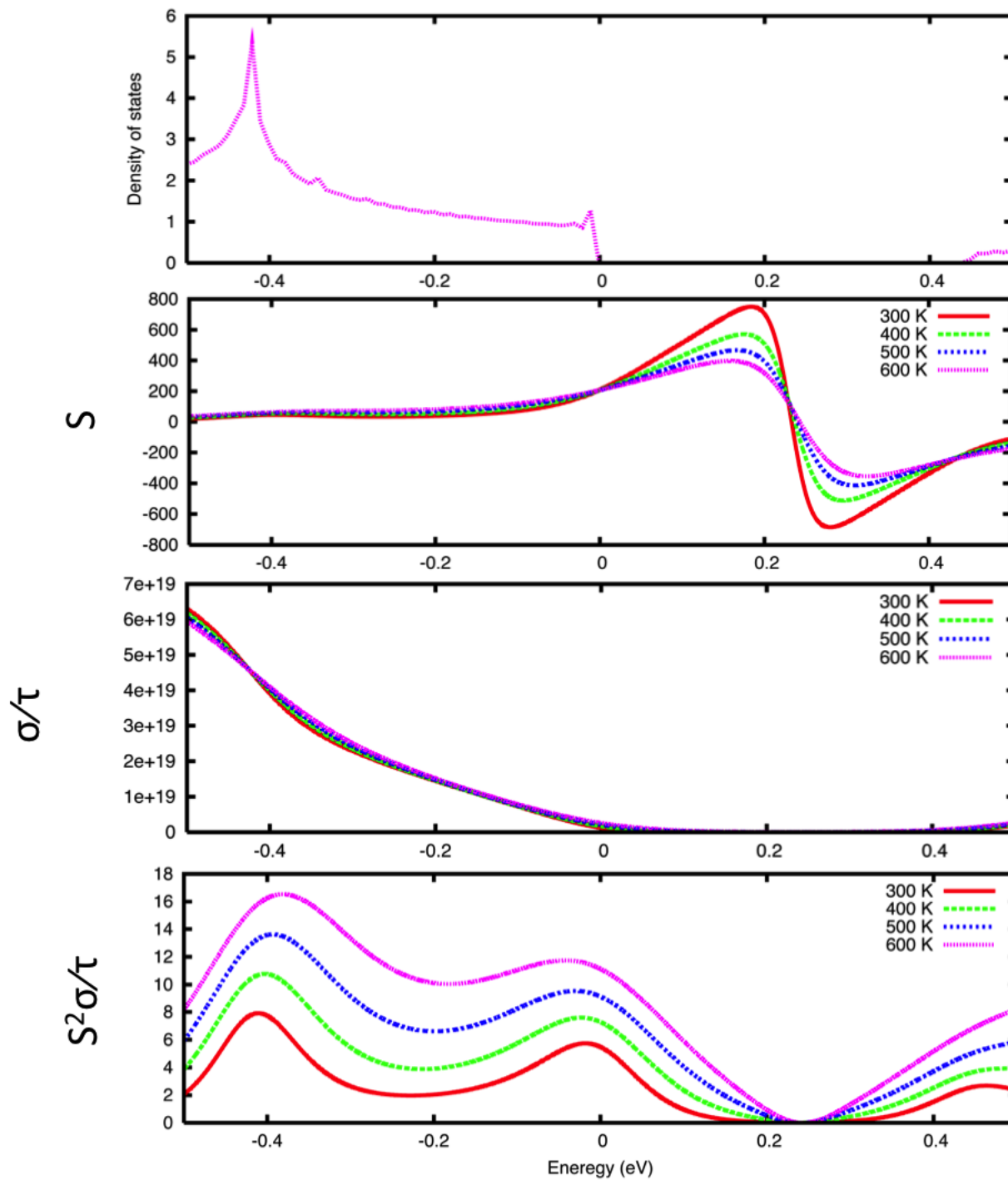
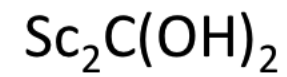
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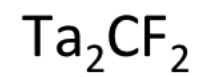




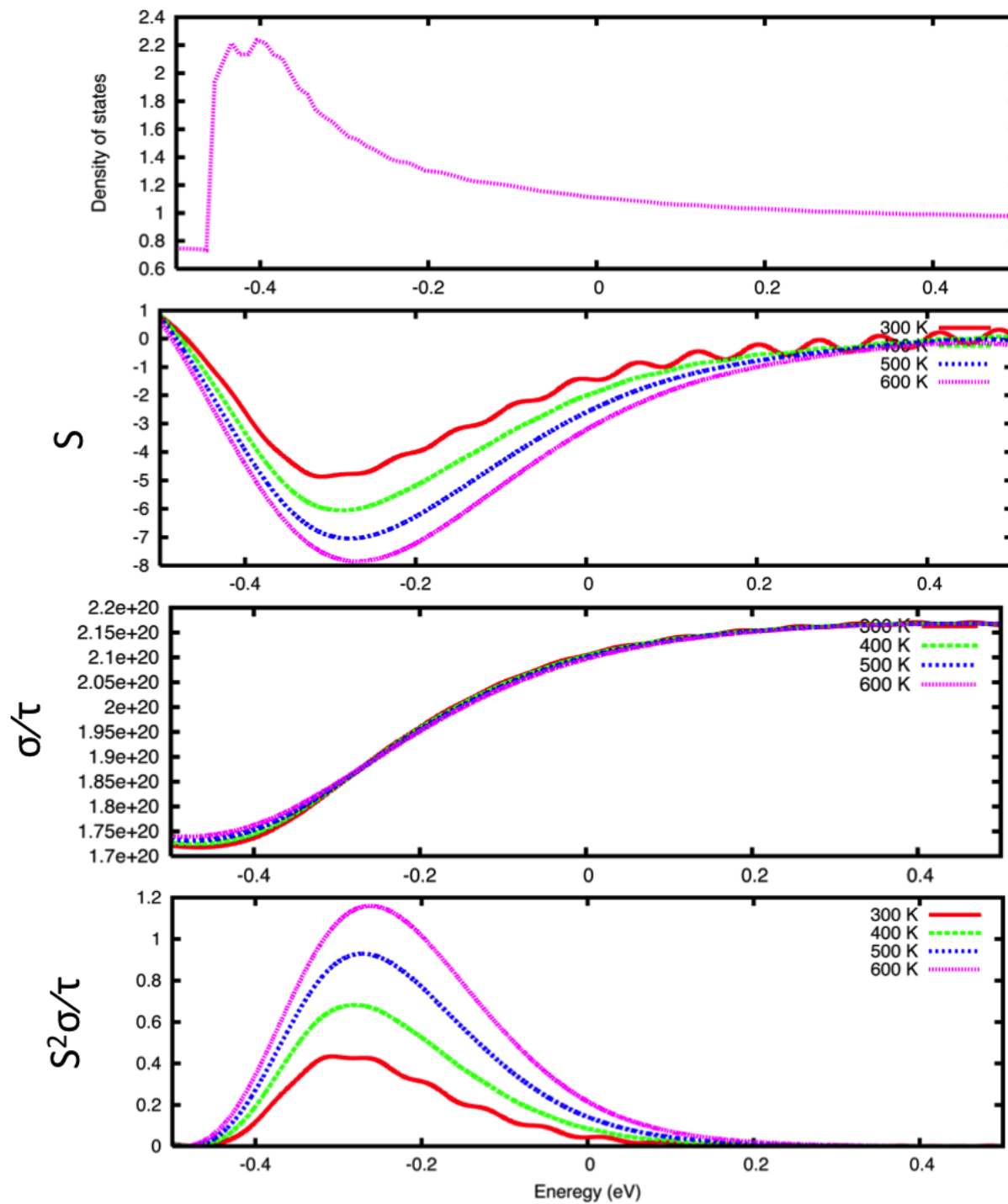
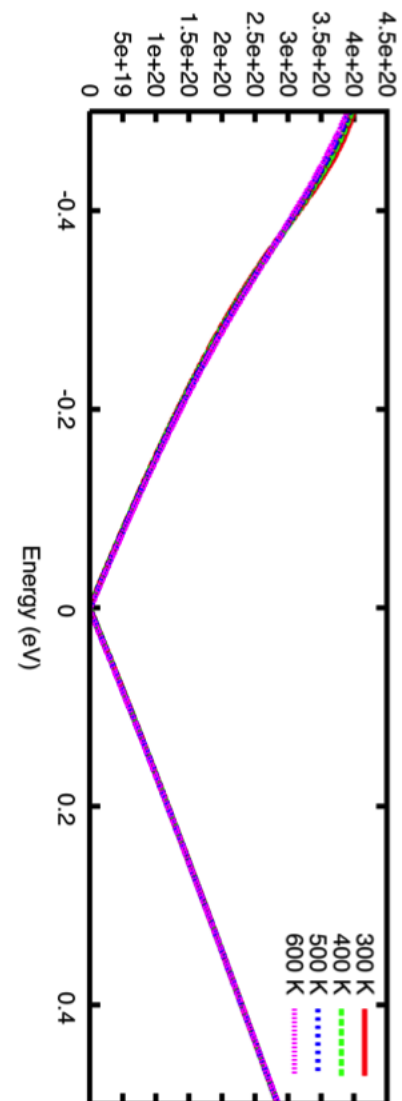


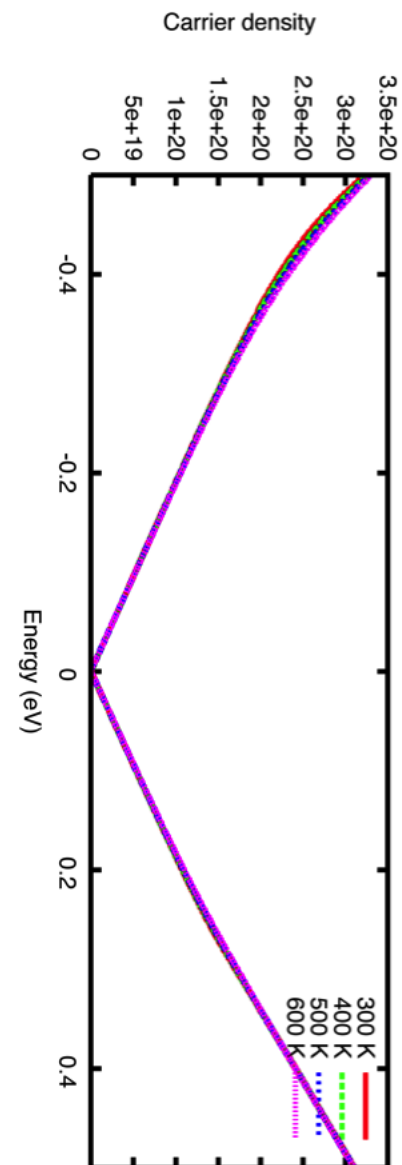
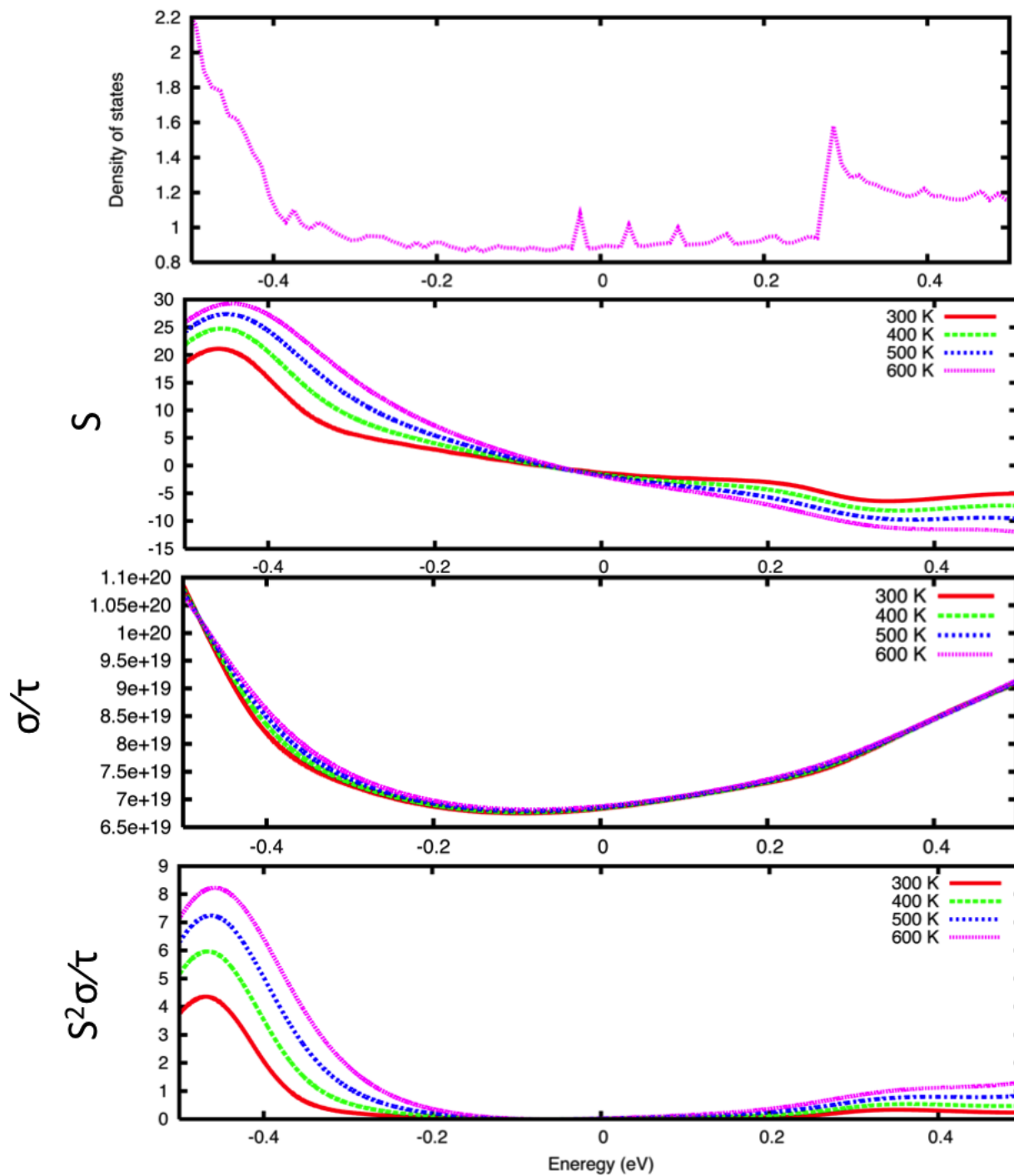
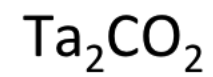


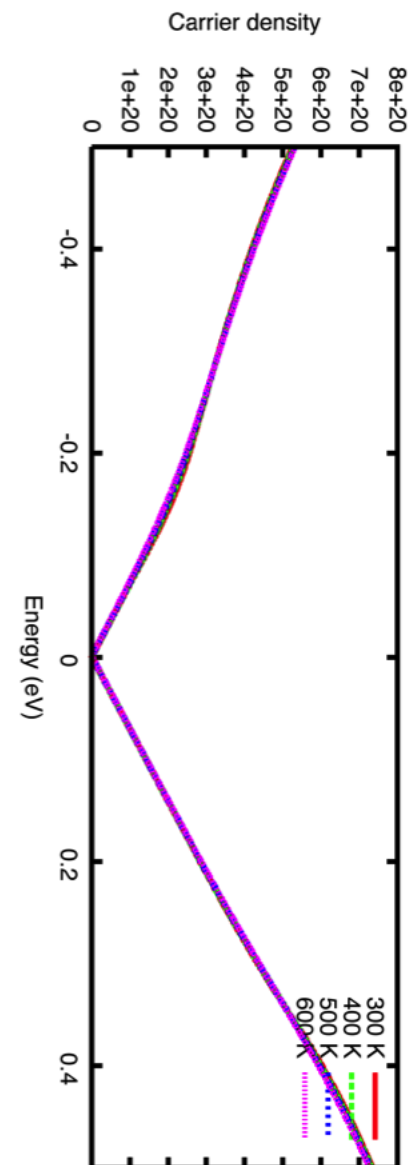
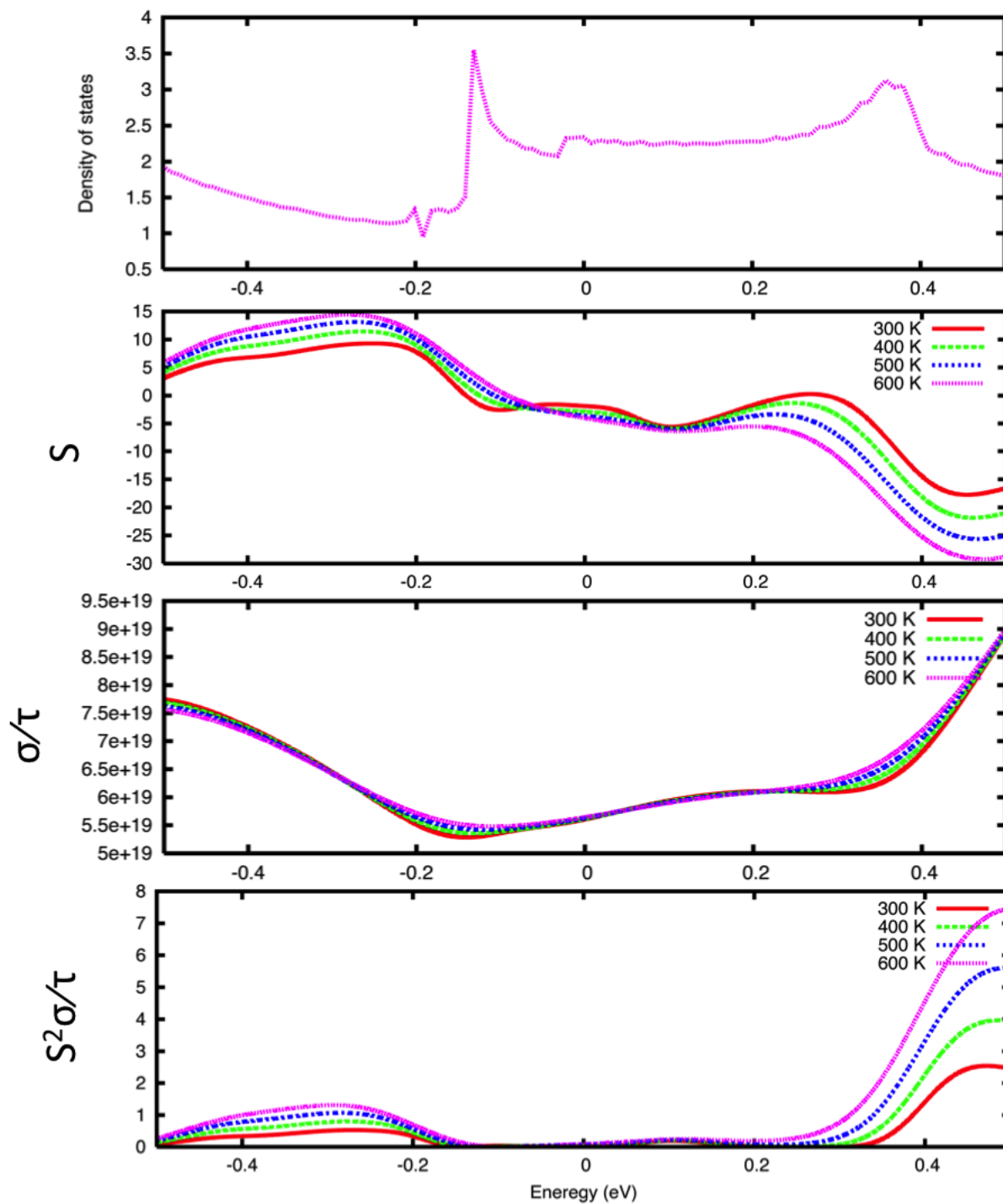
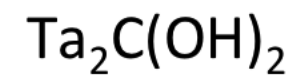


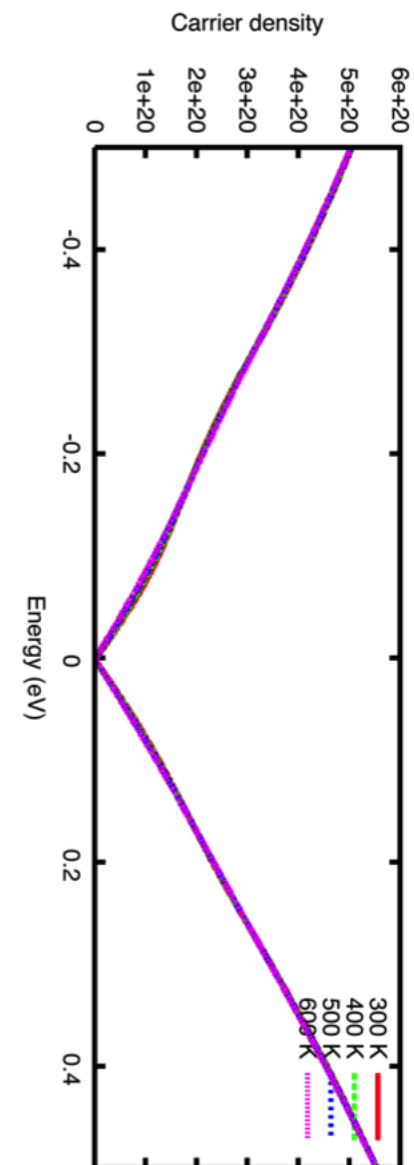
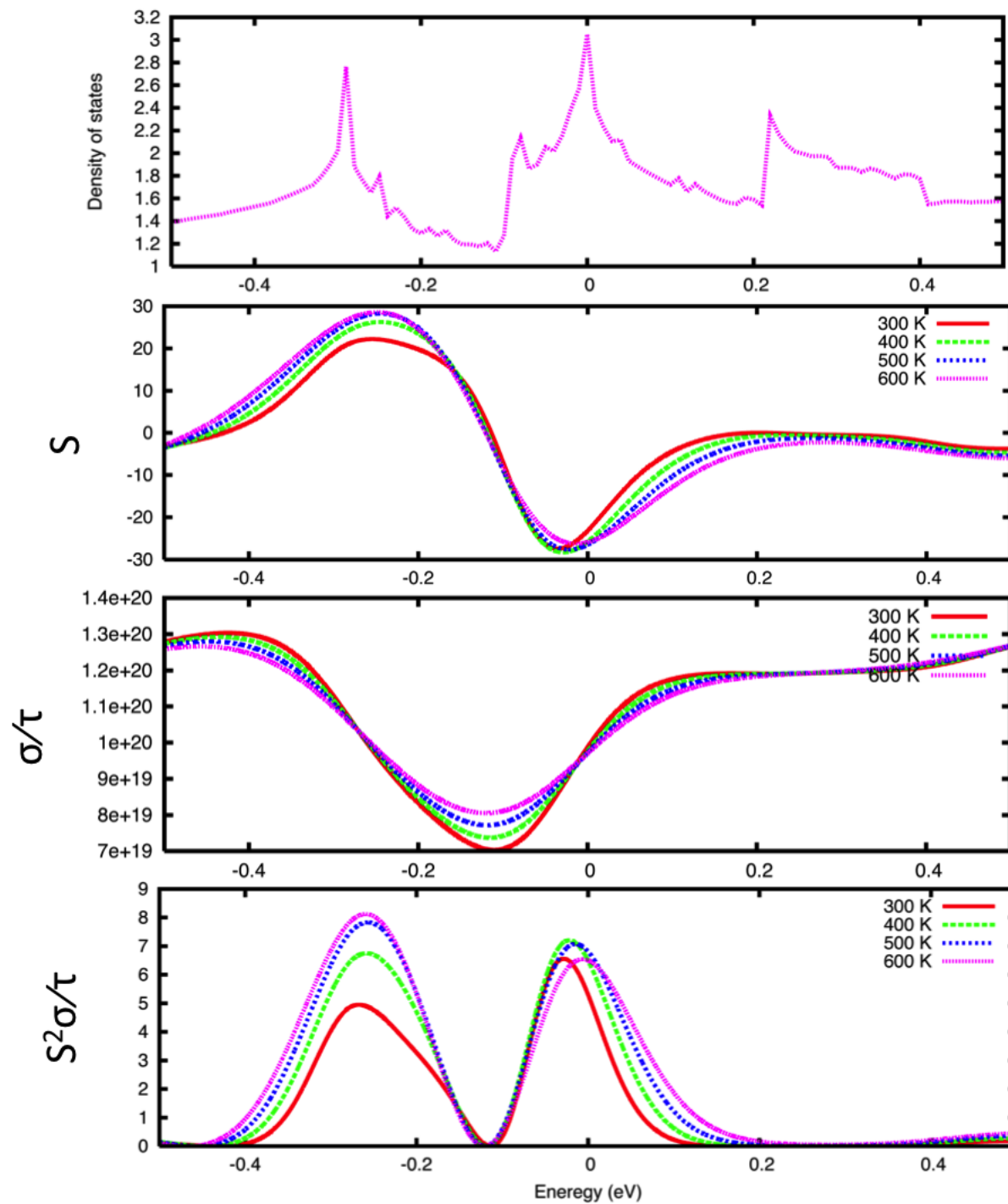
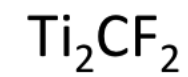


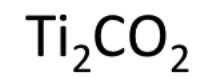
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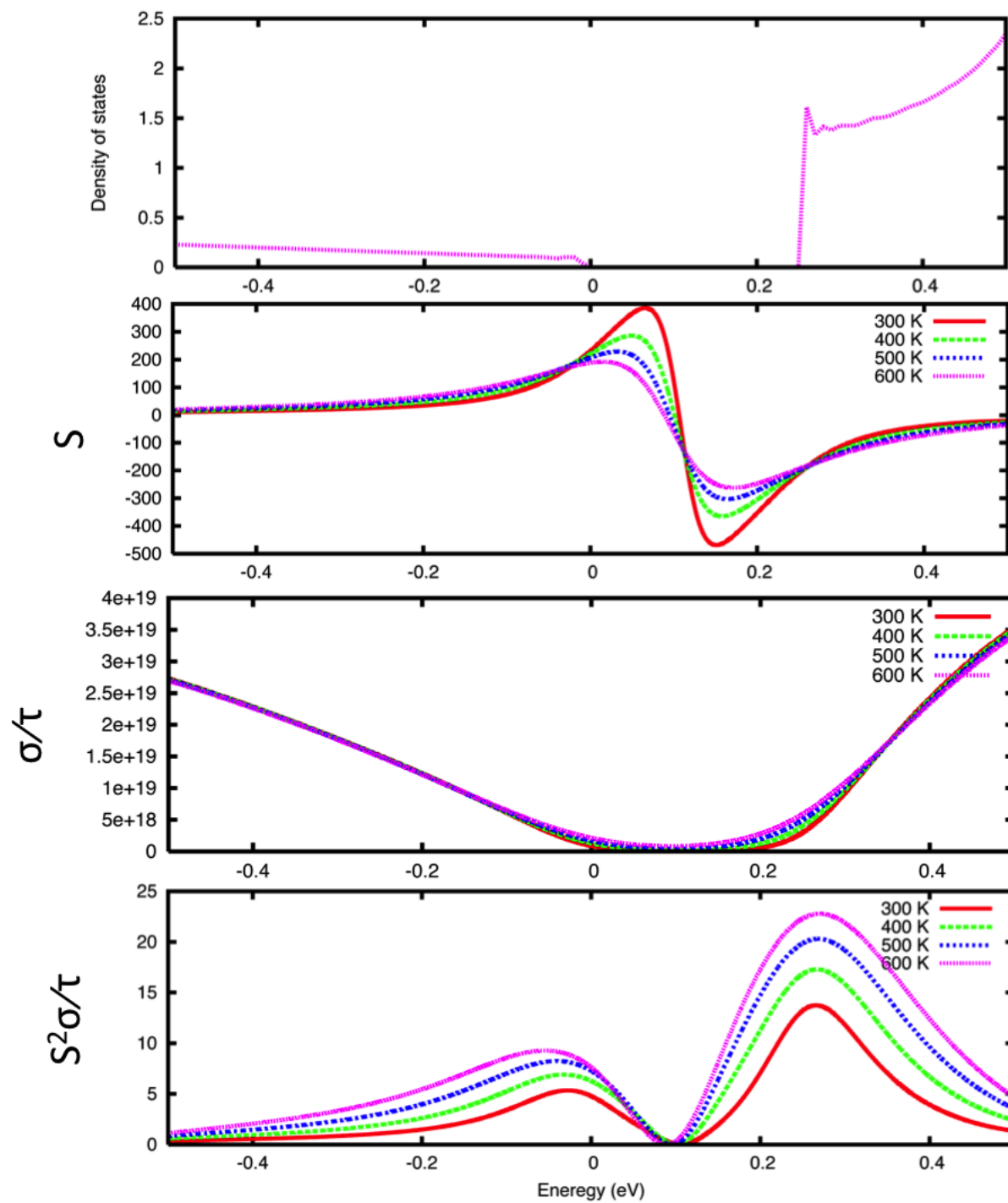
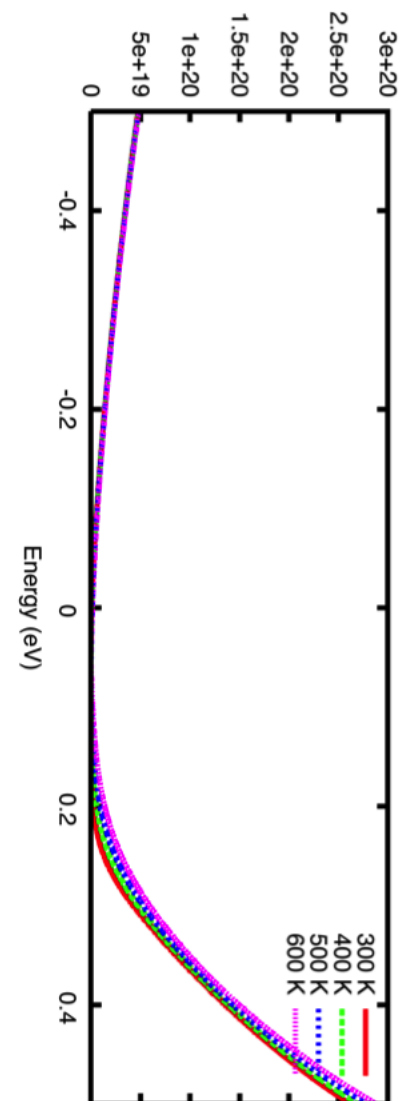


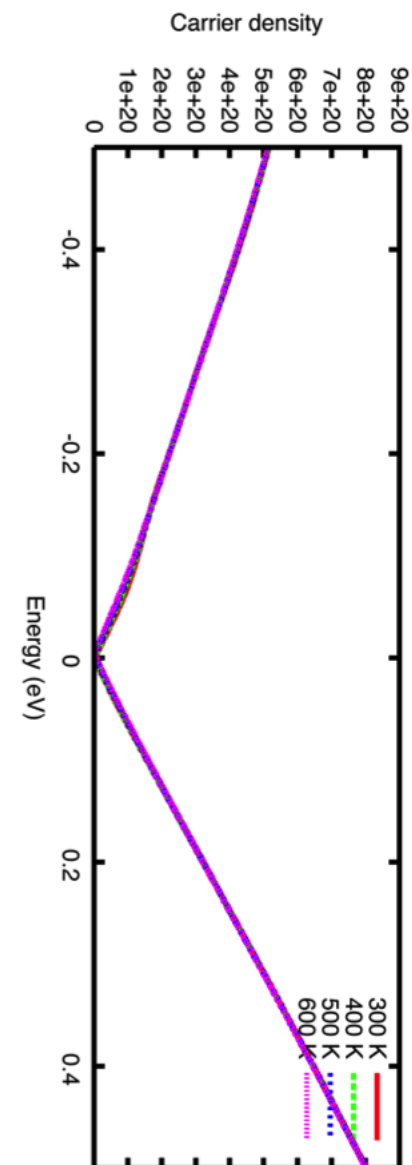
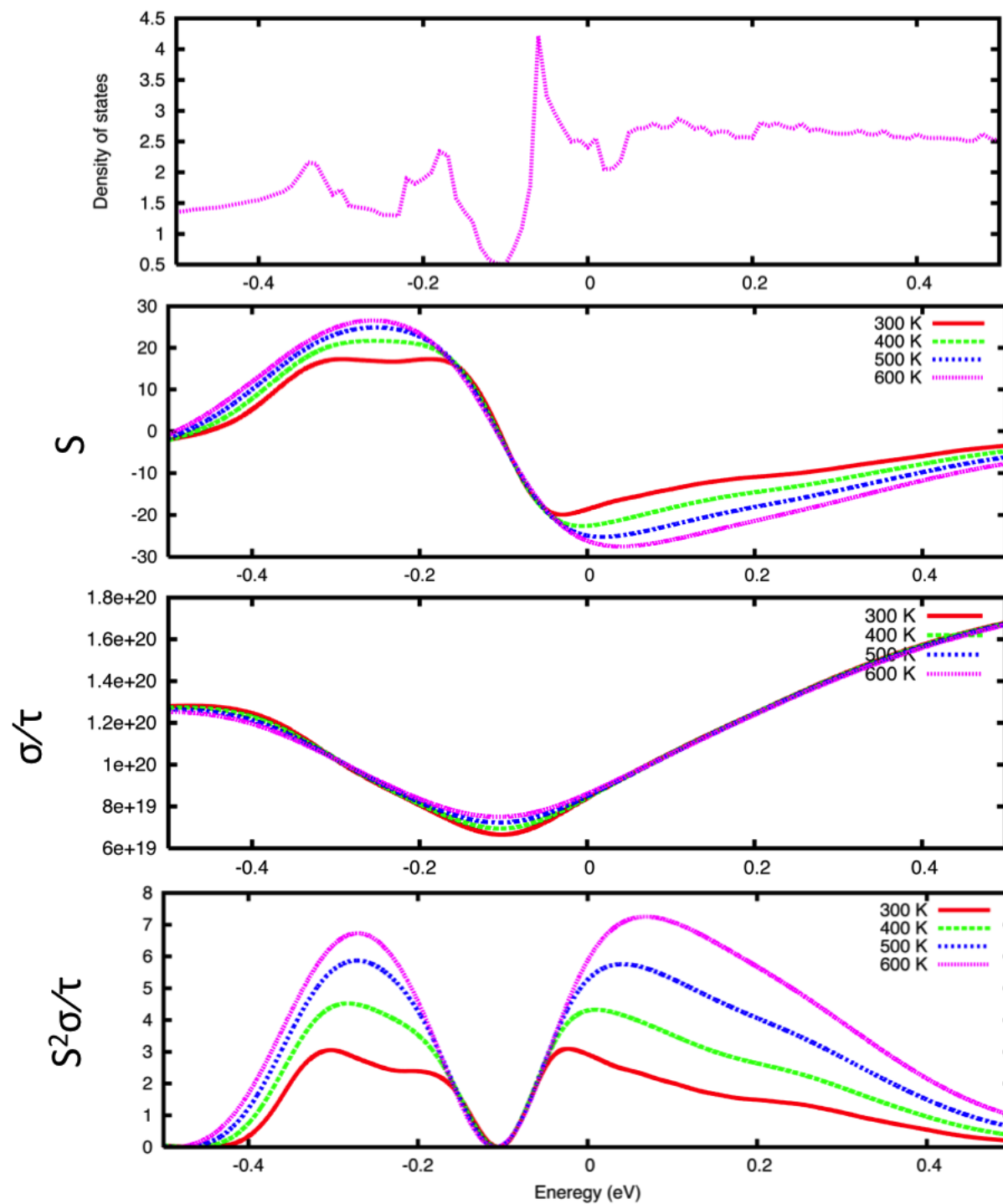
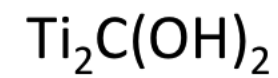


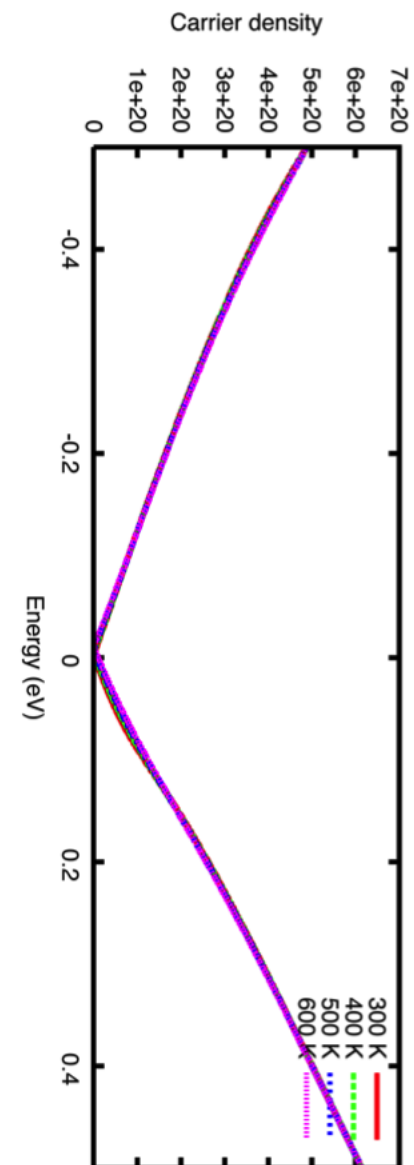
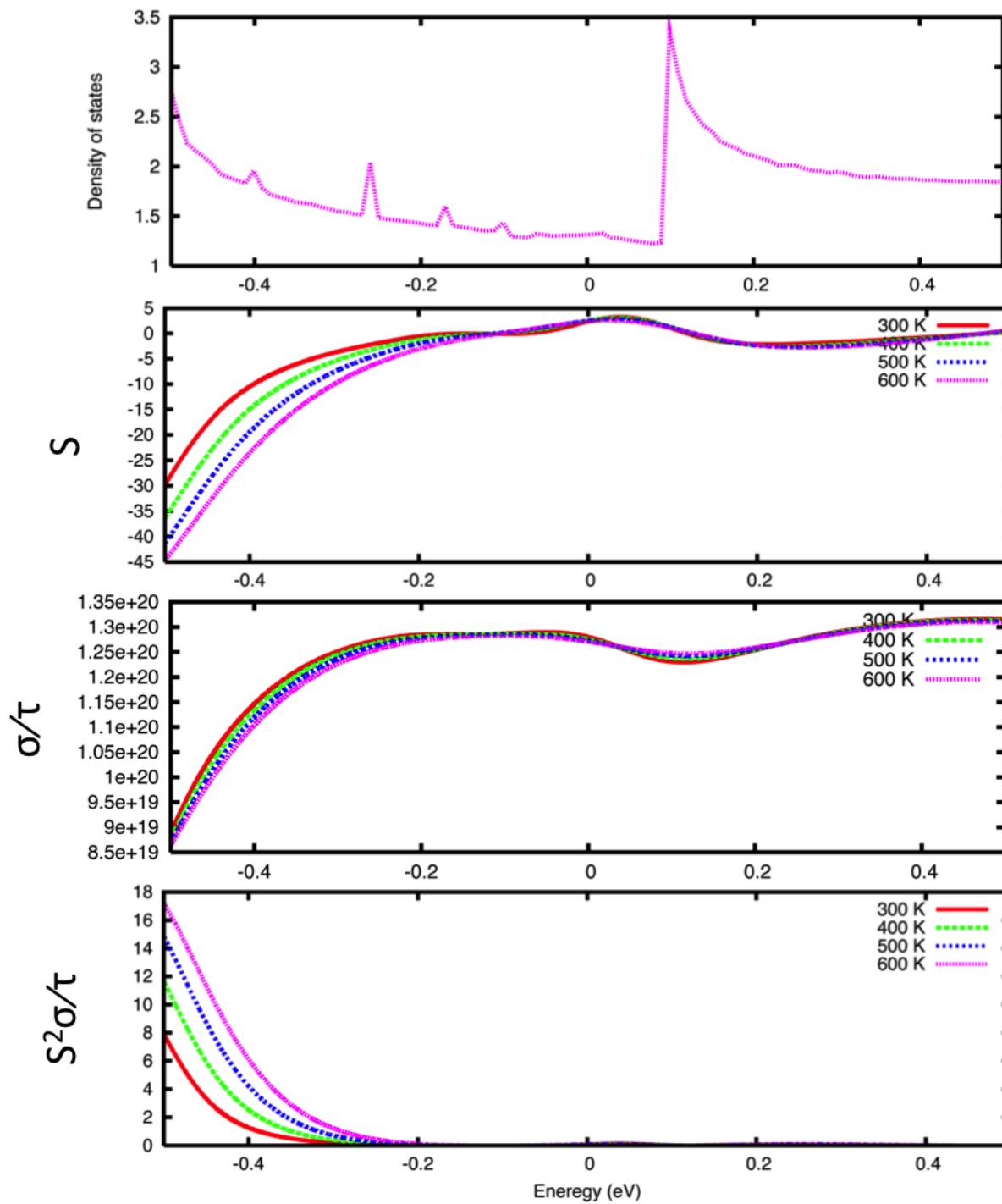
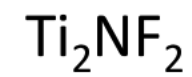


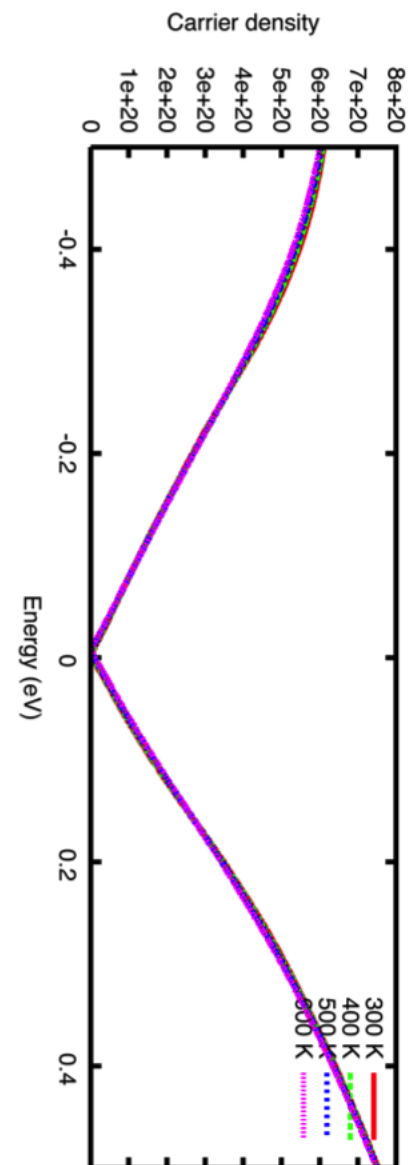
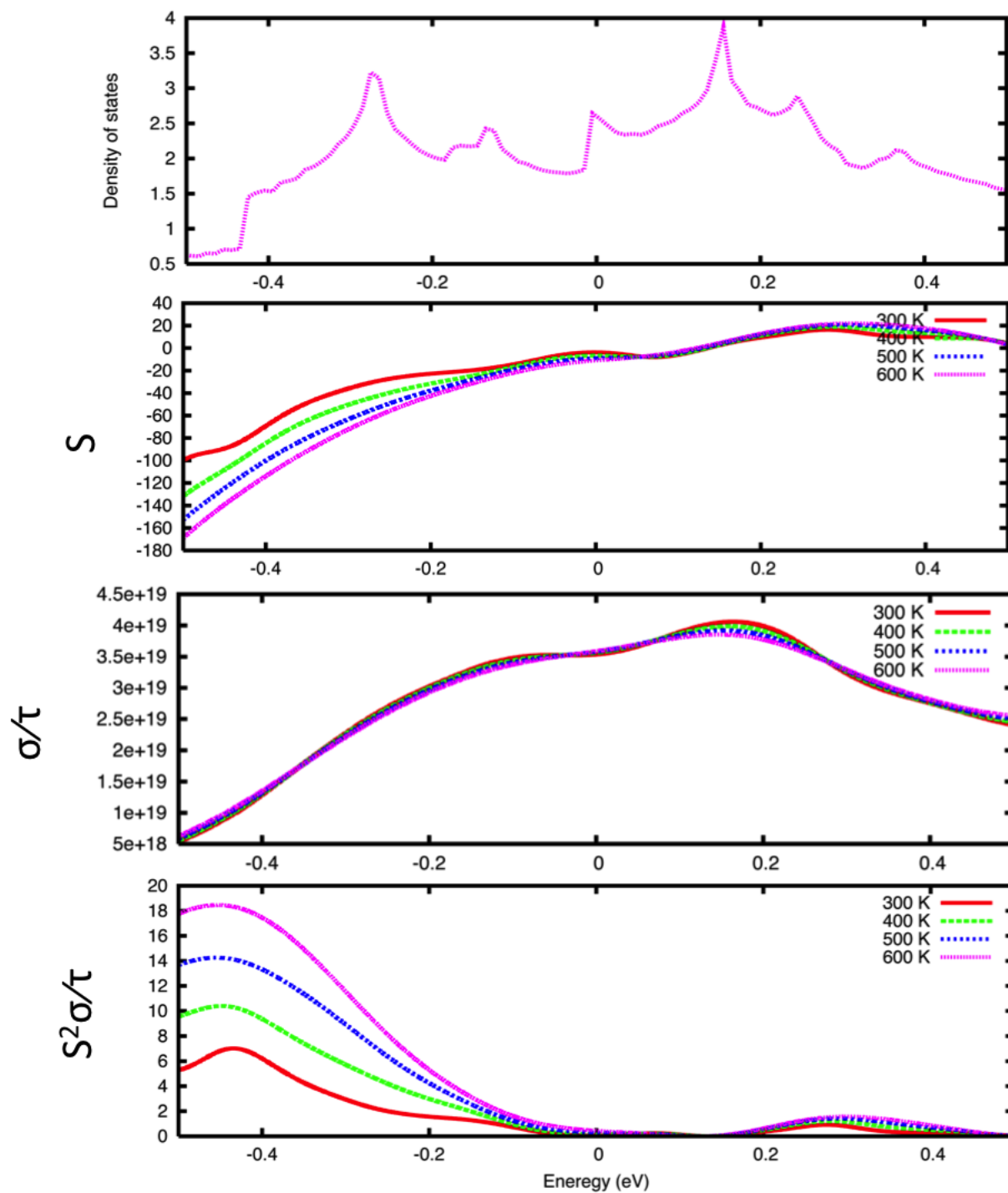
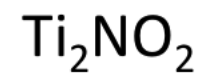


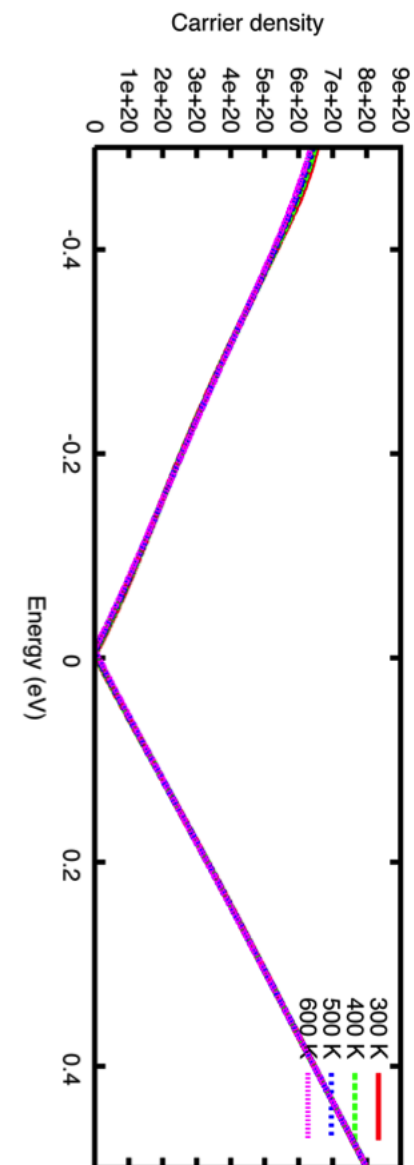
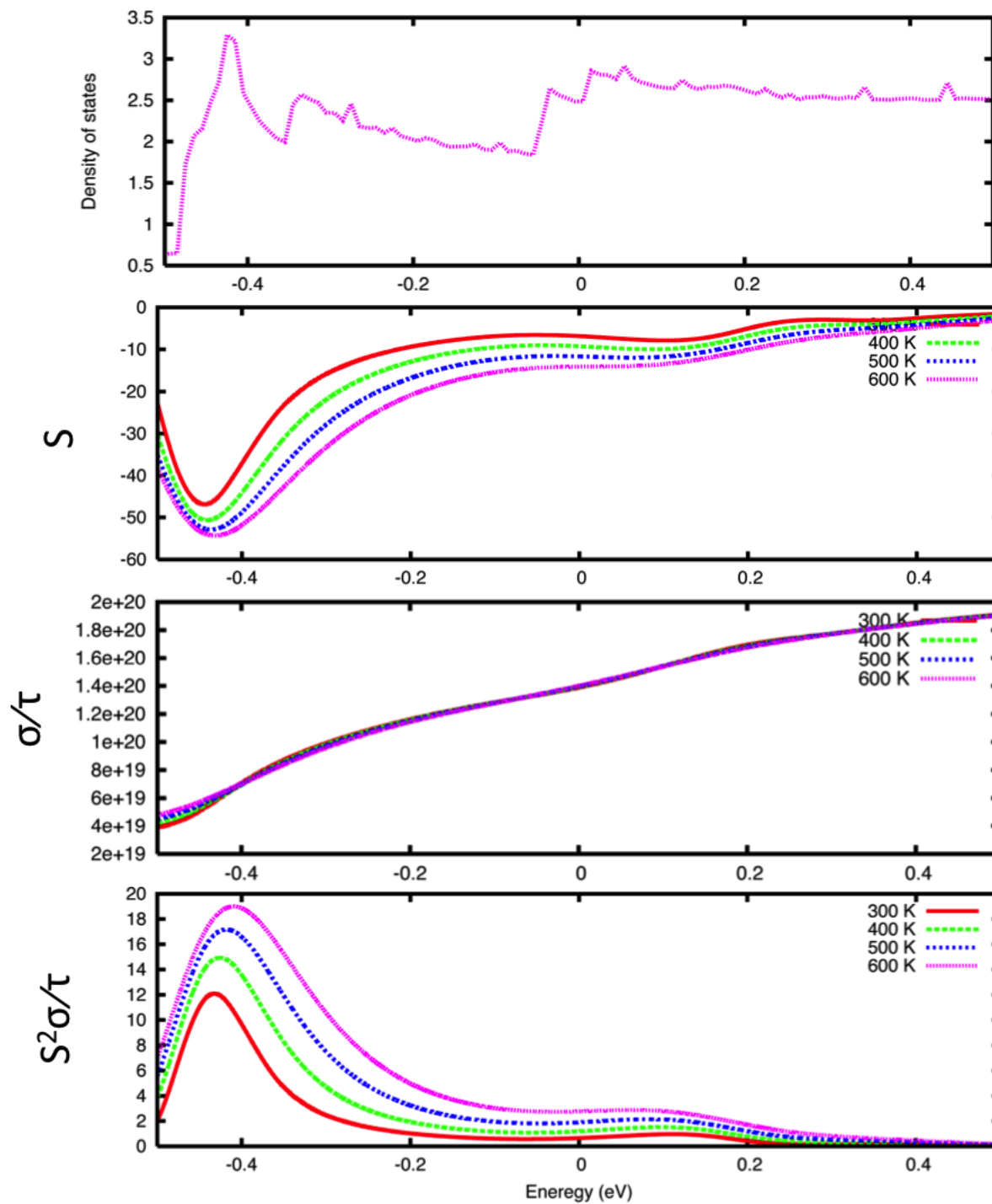
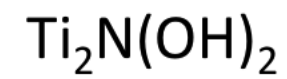
Carrier density

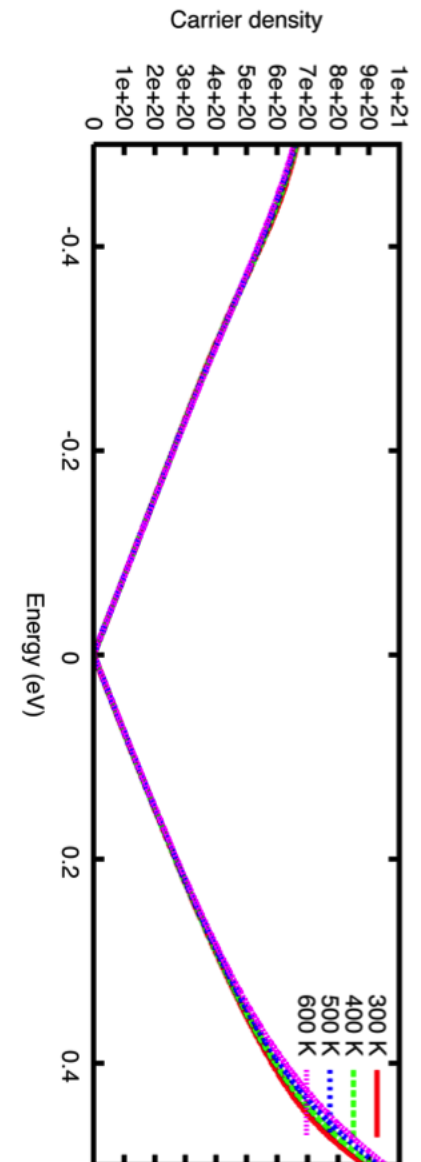
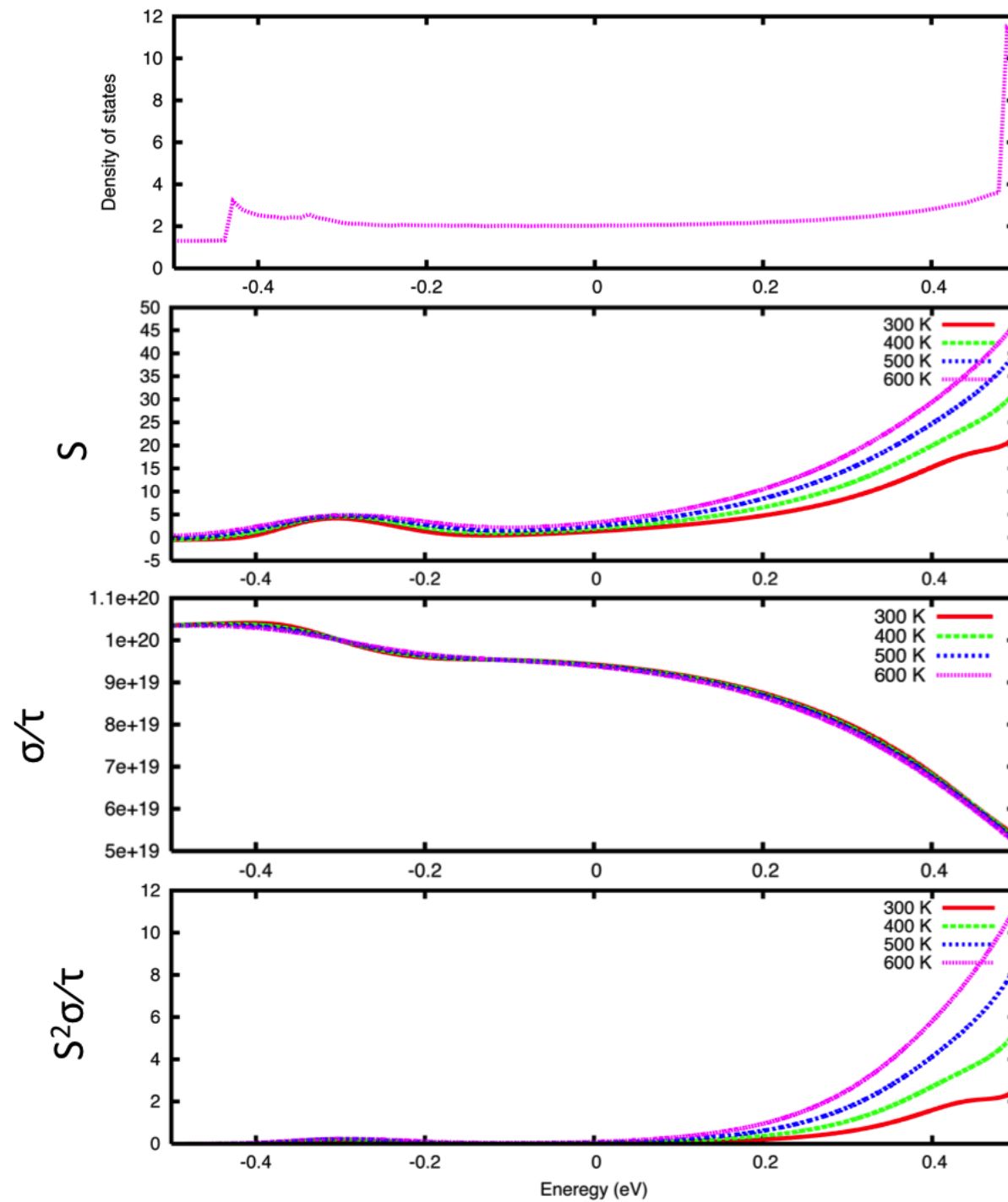
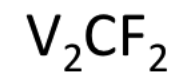


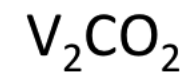




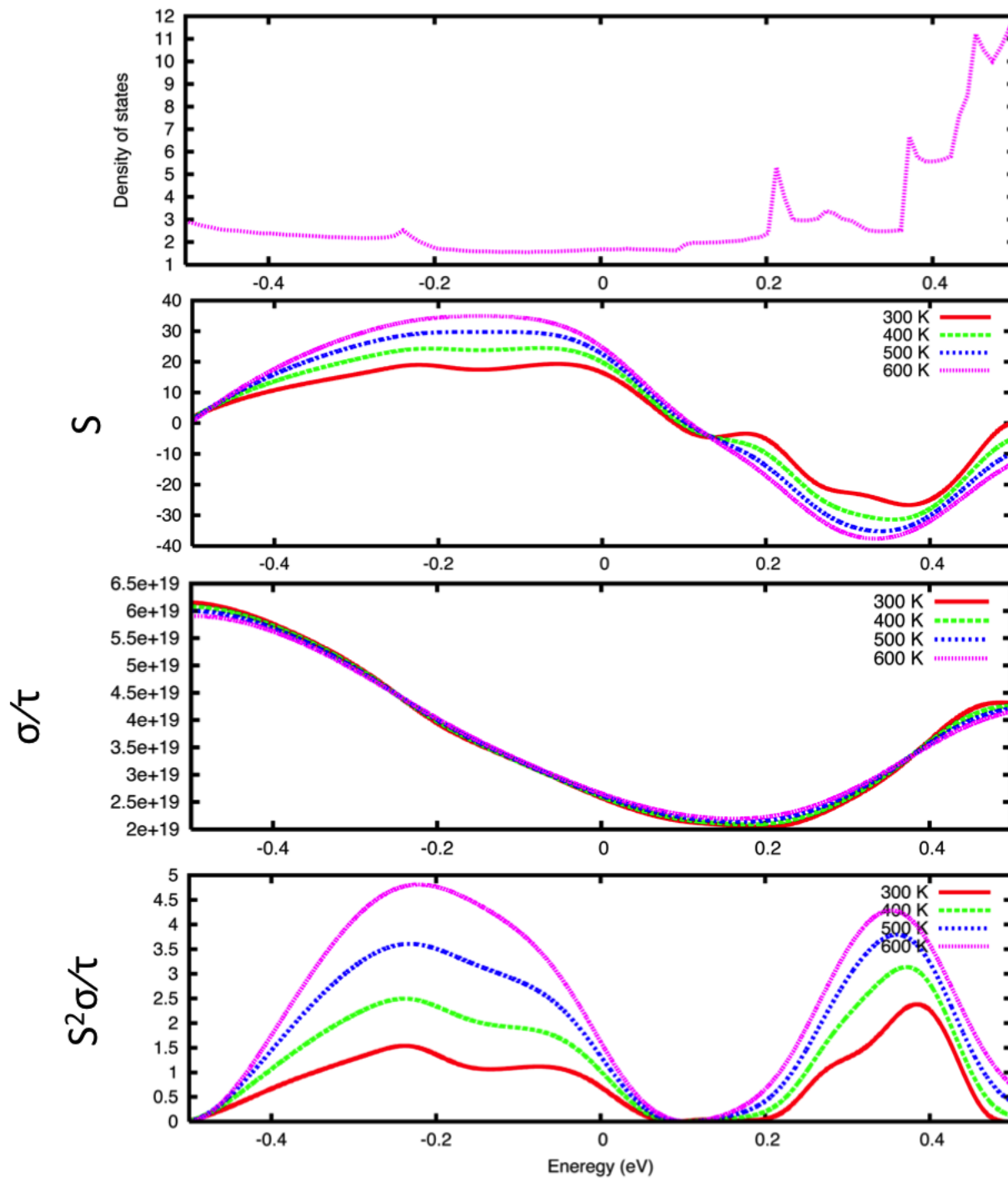
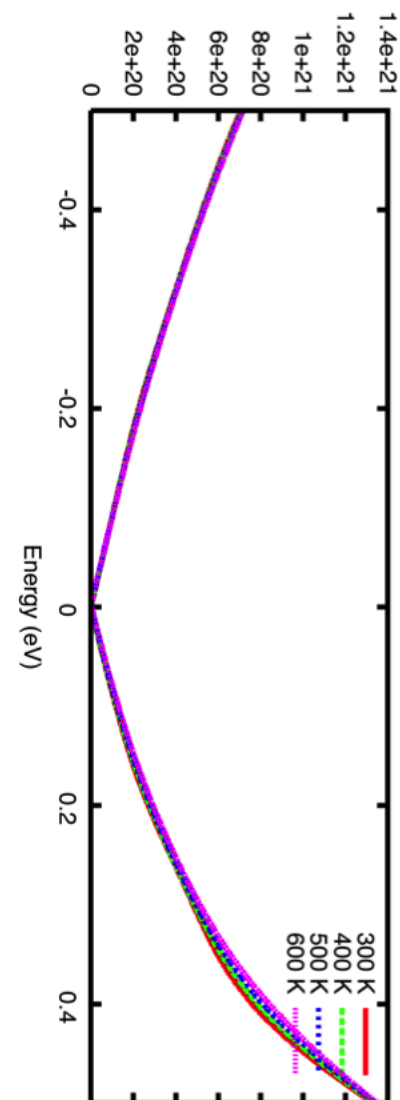


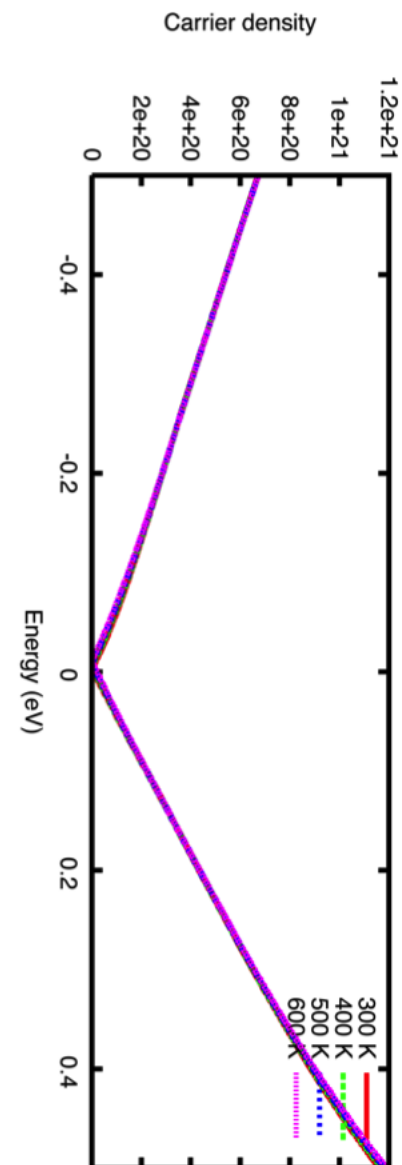
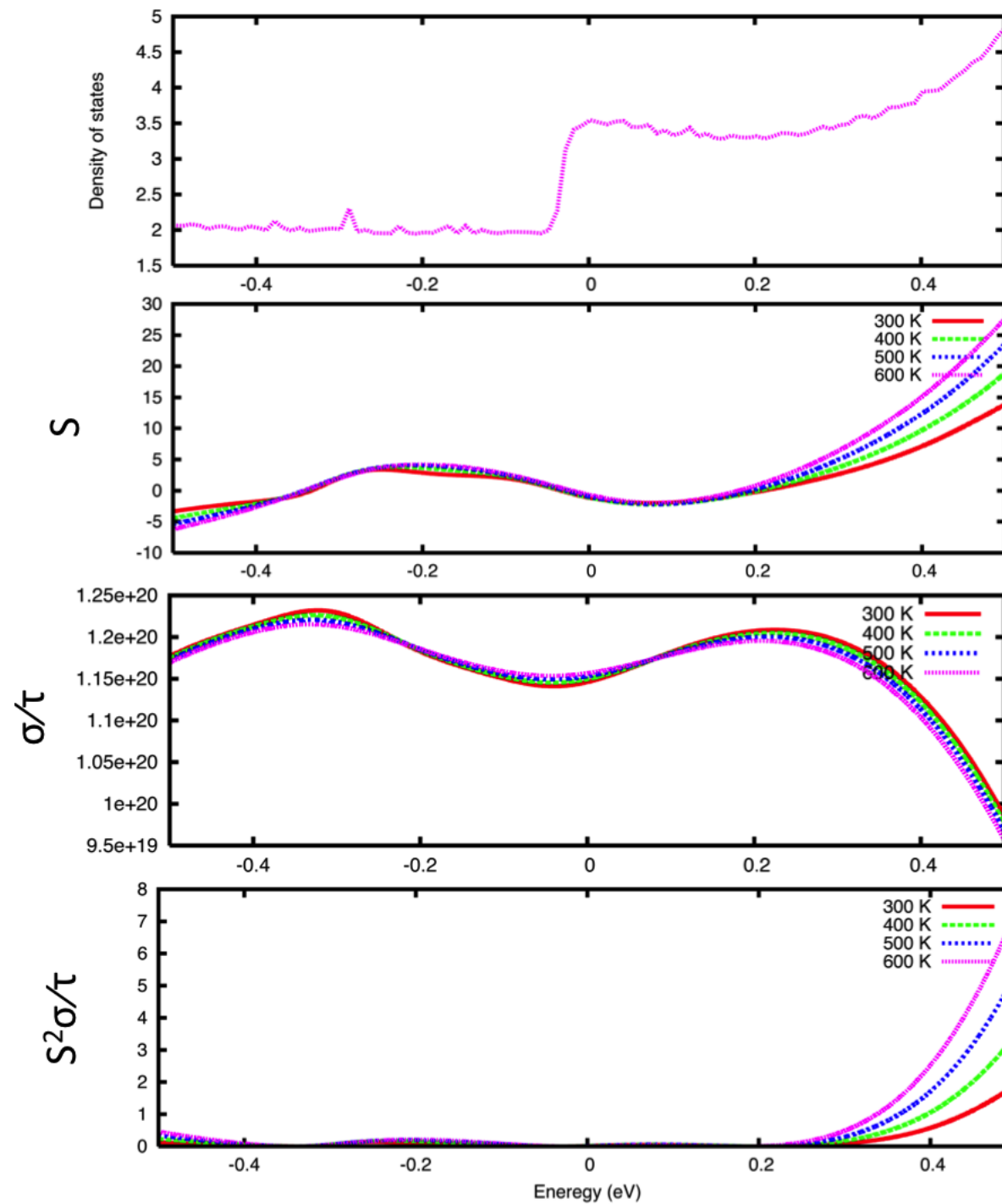
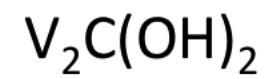


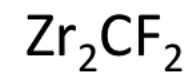




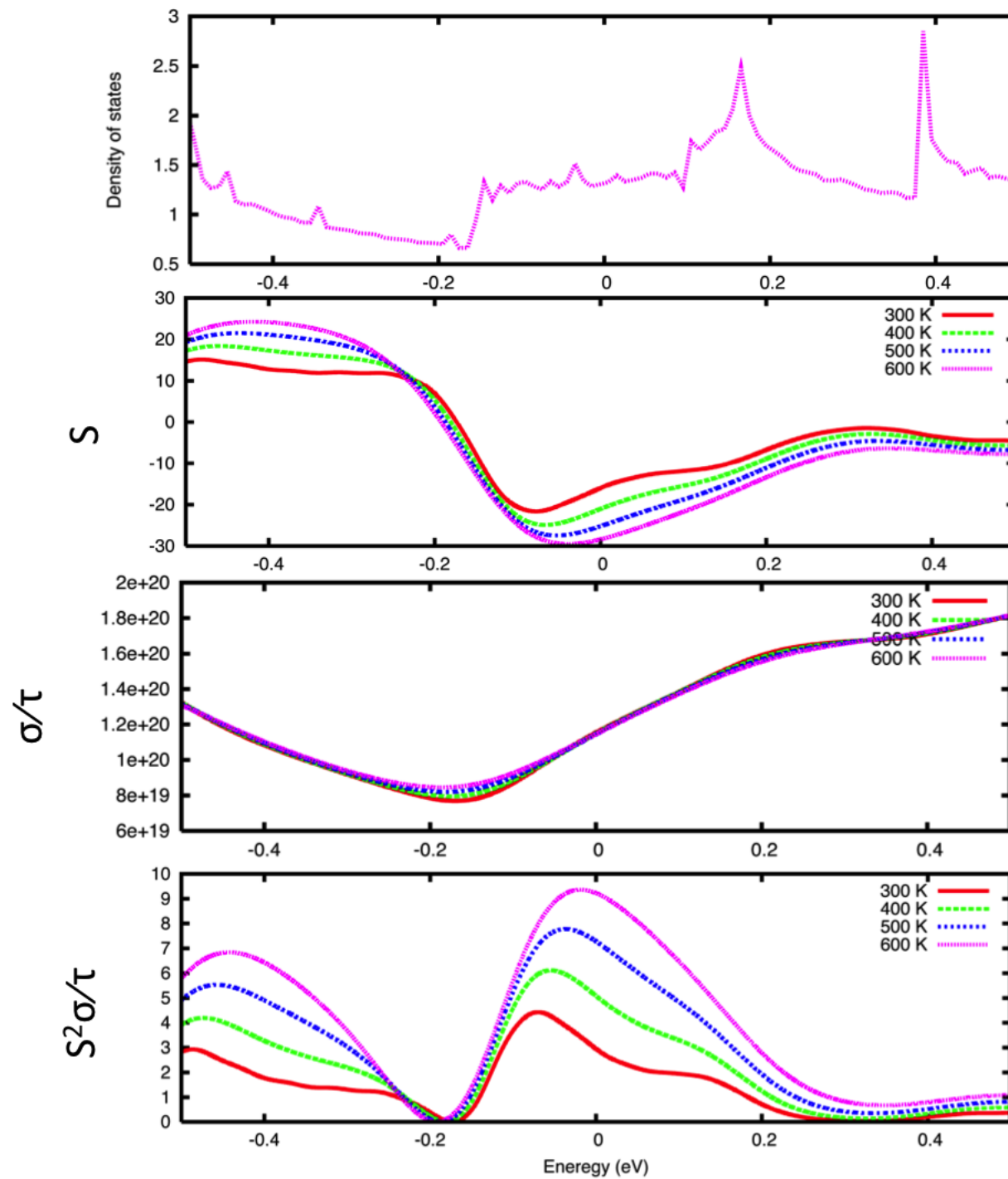
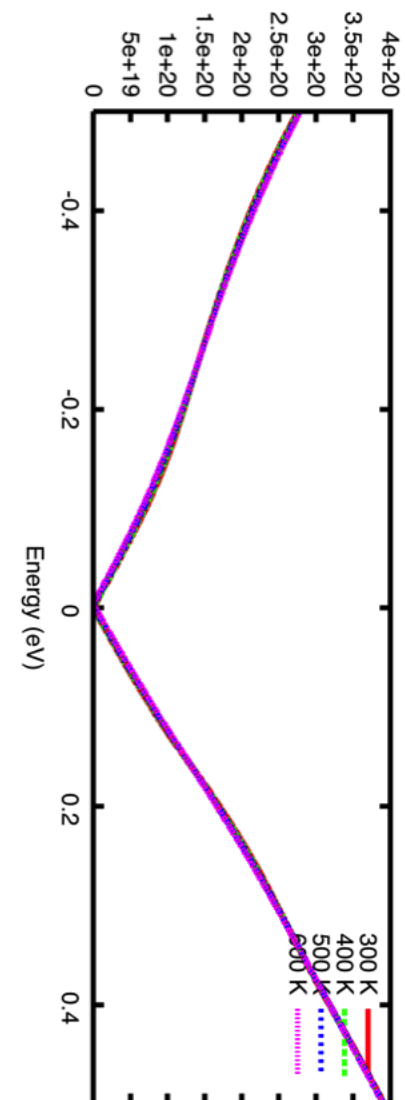
Carrier density

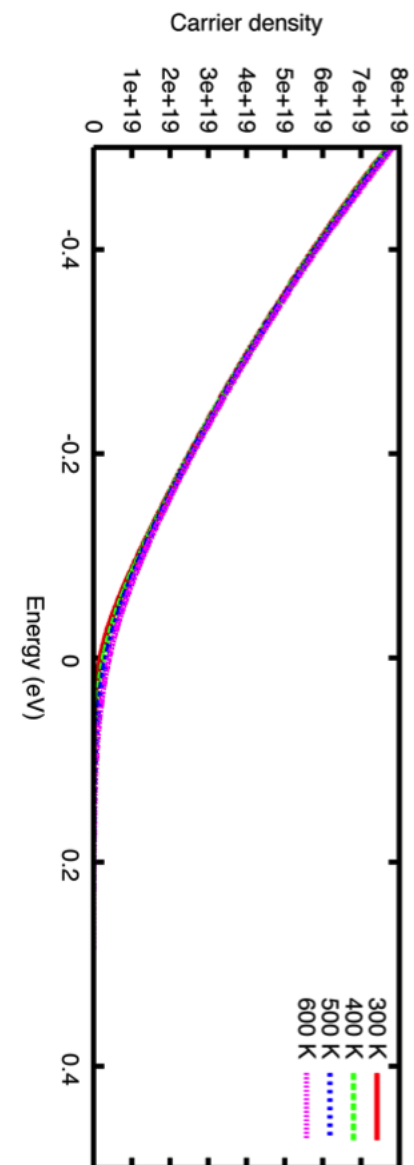
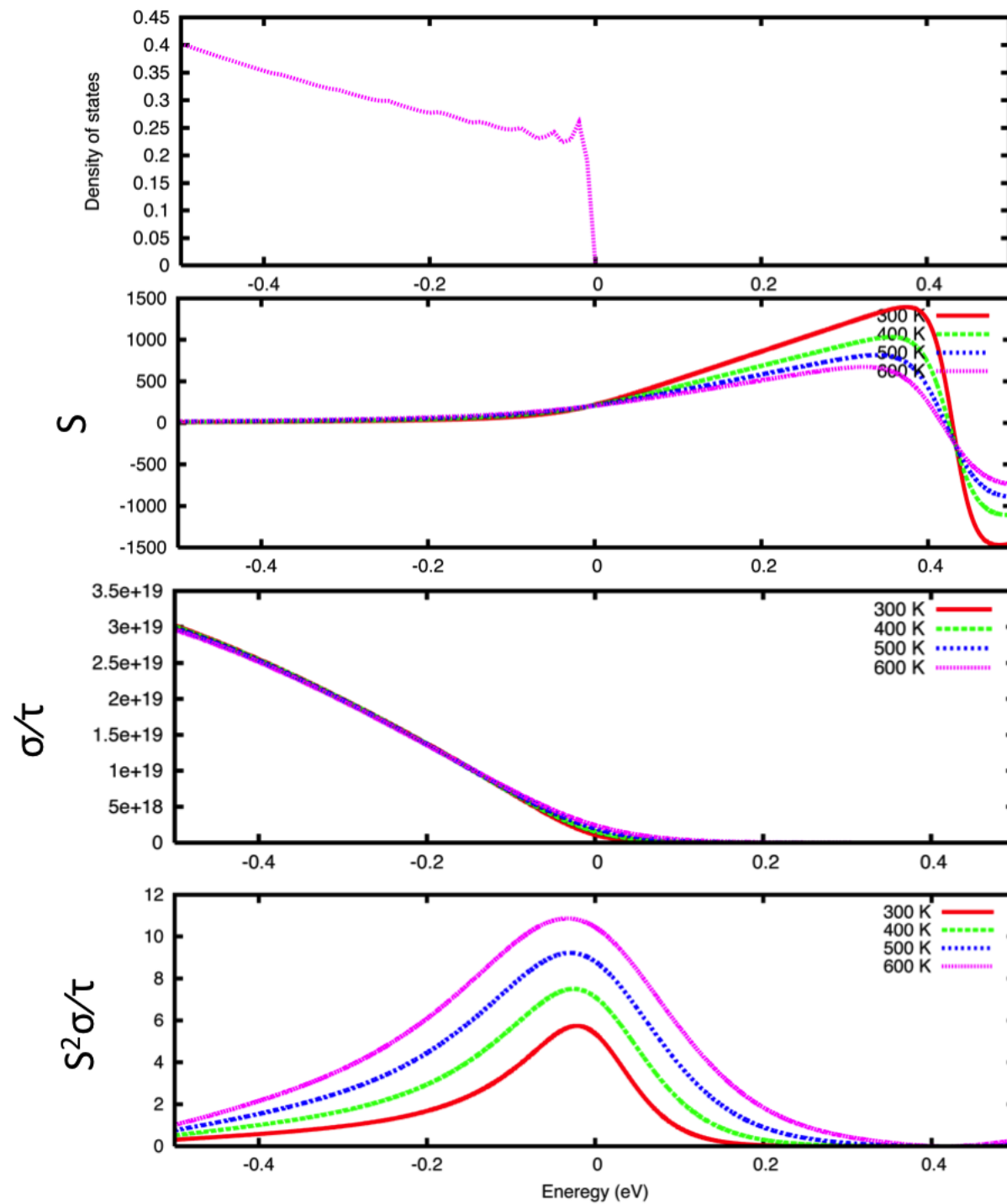
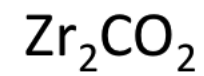


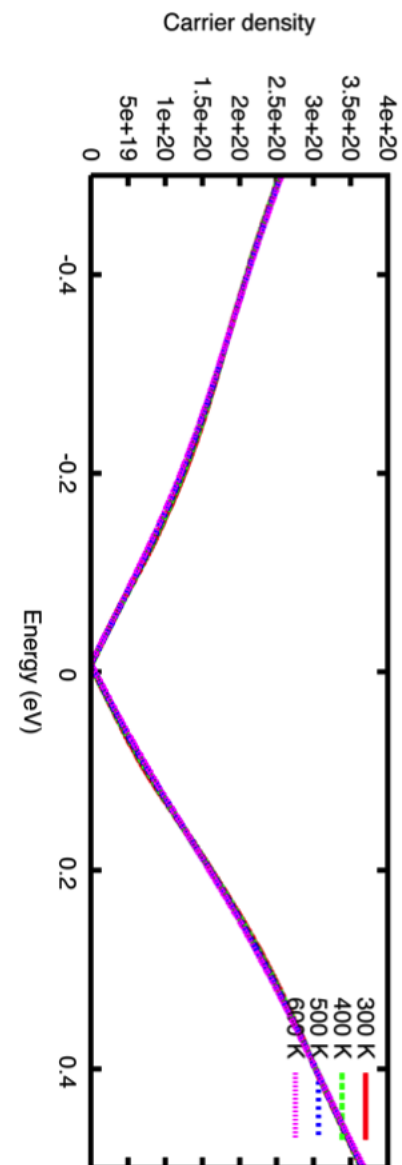
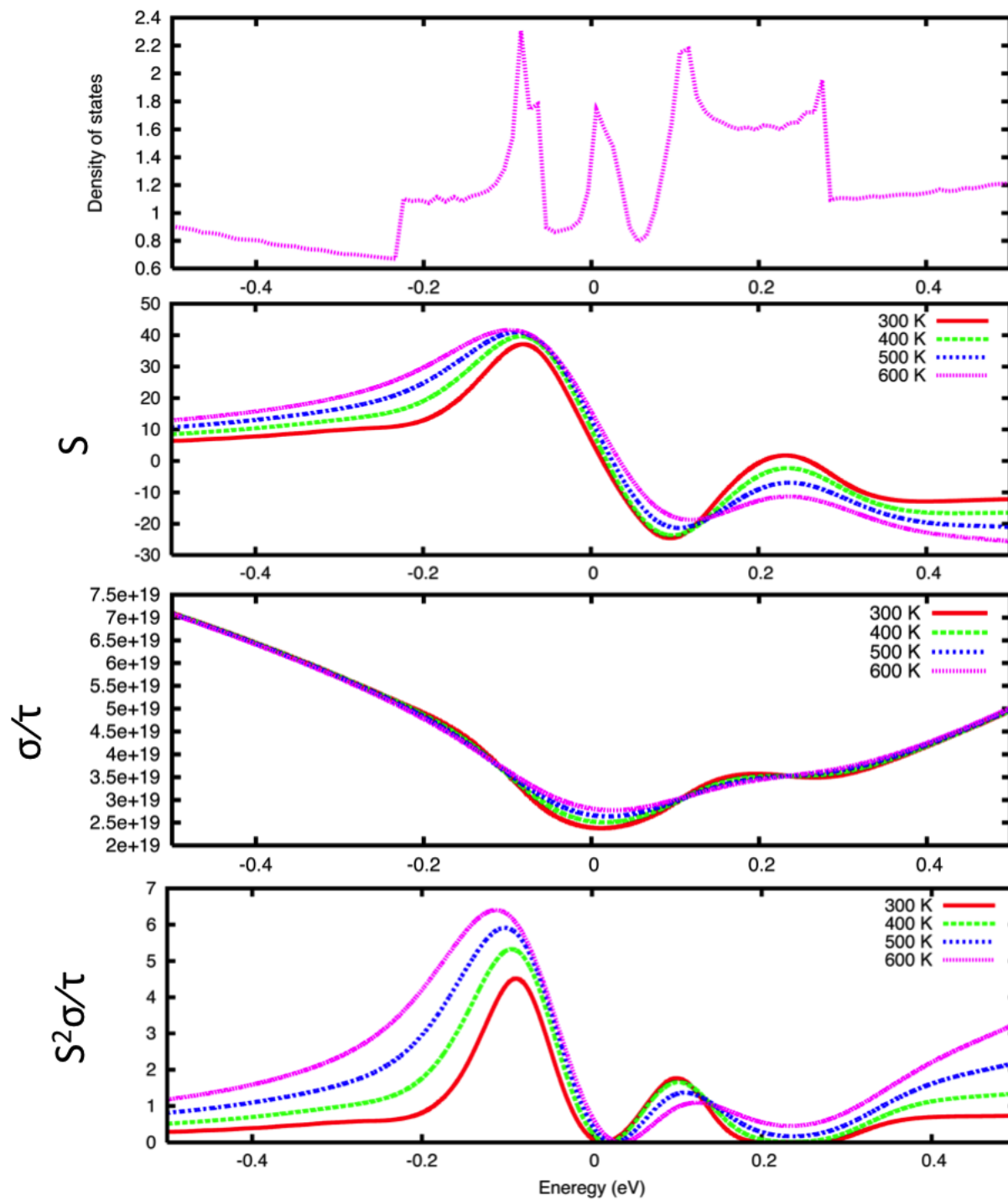
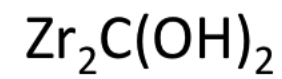


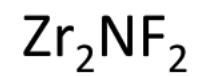


Carrier density

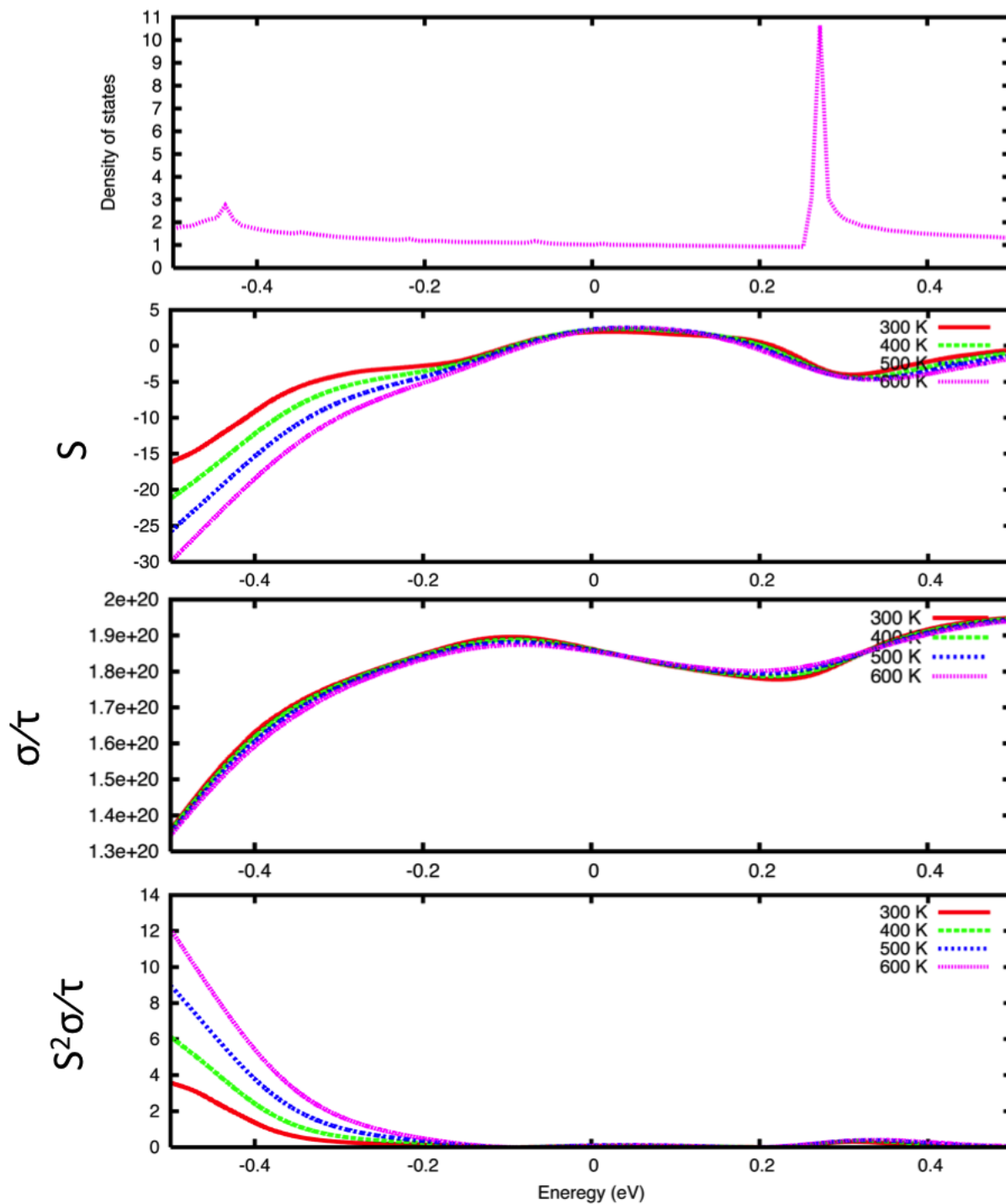
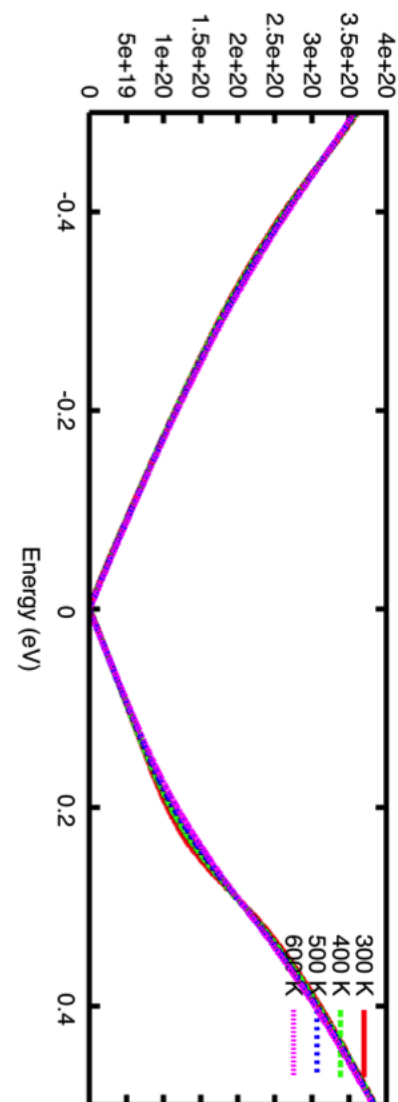


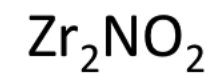




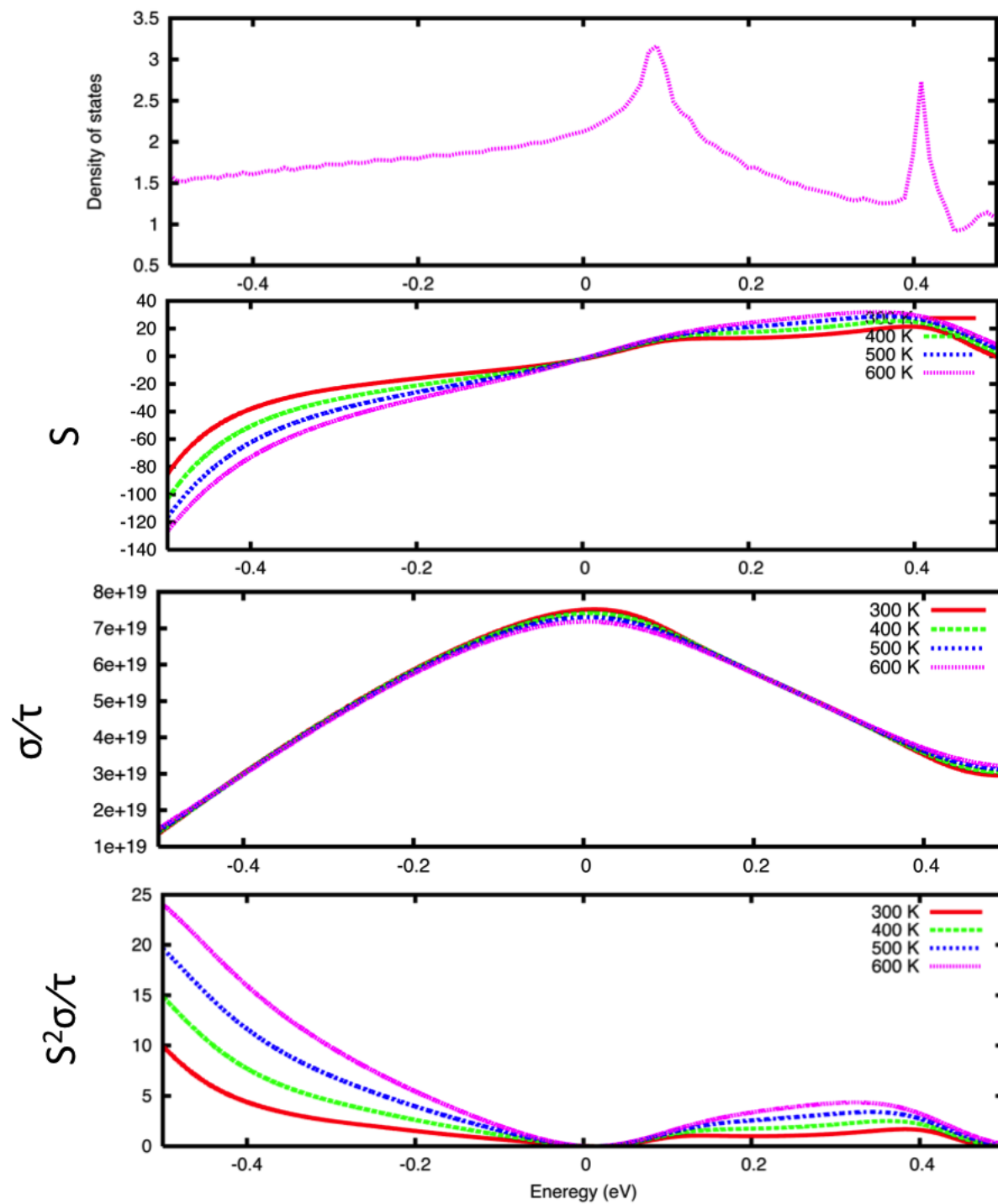
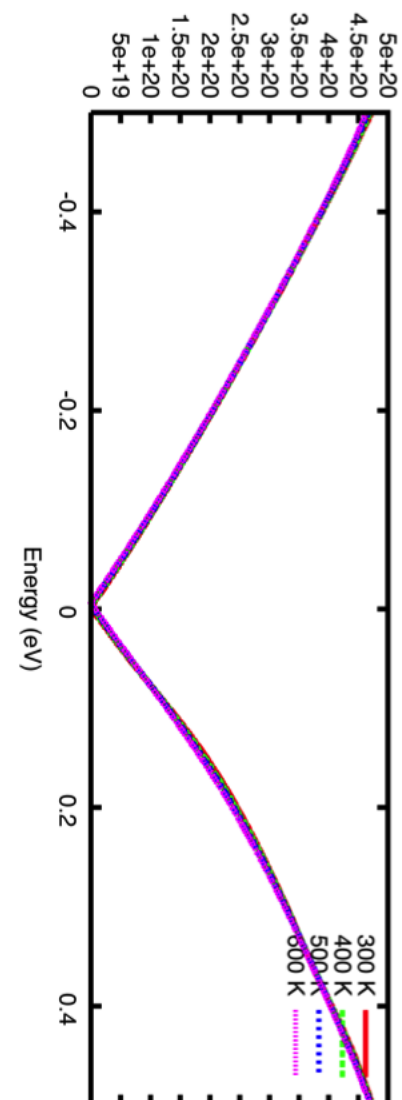


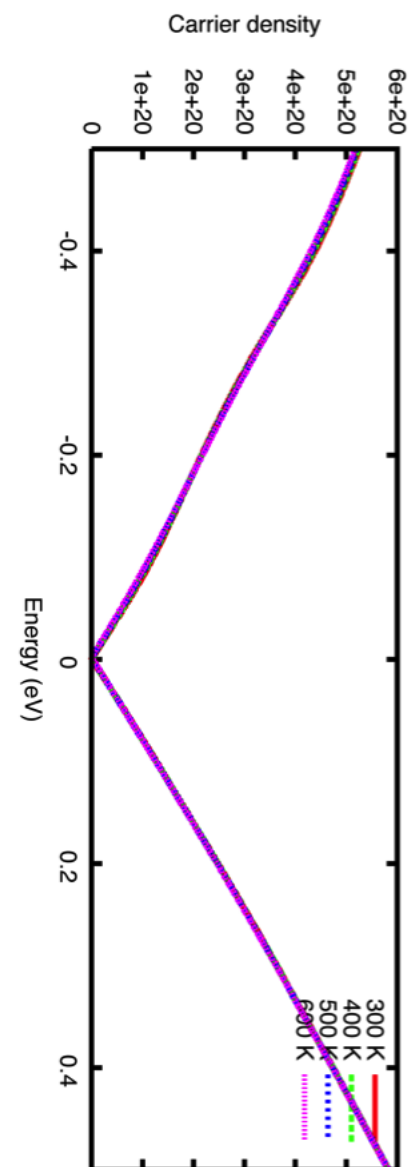
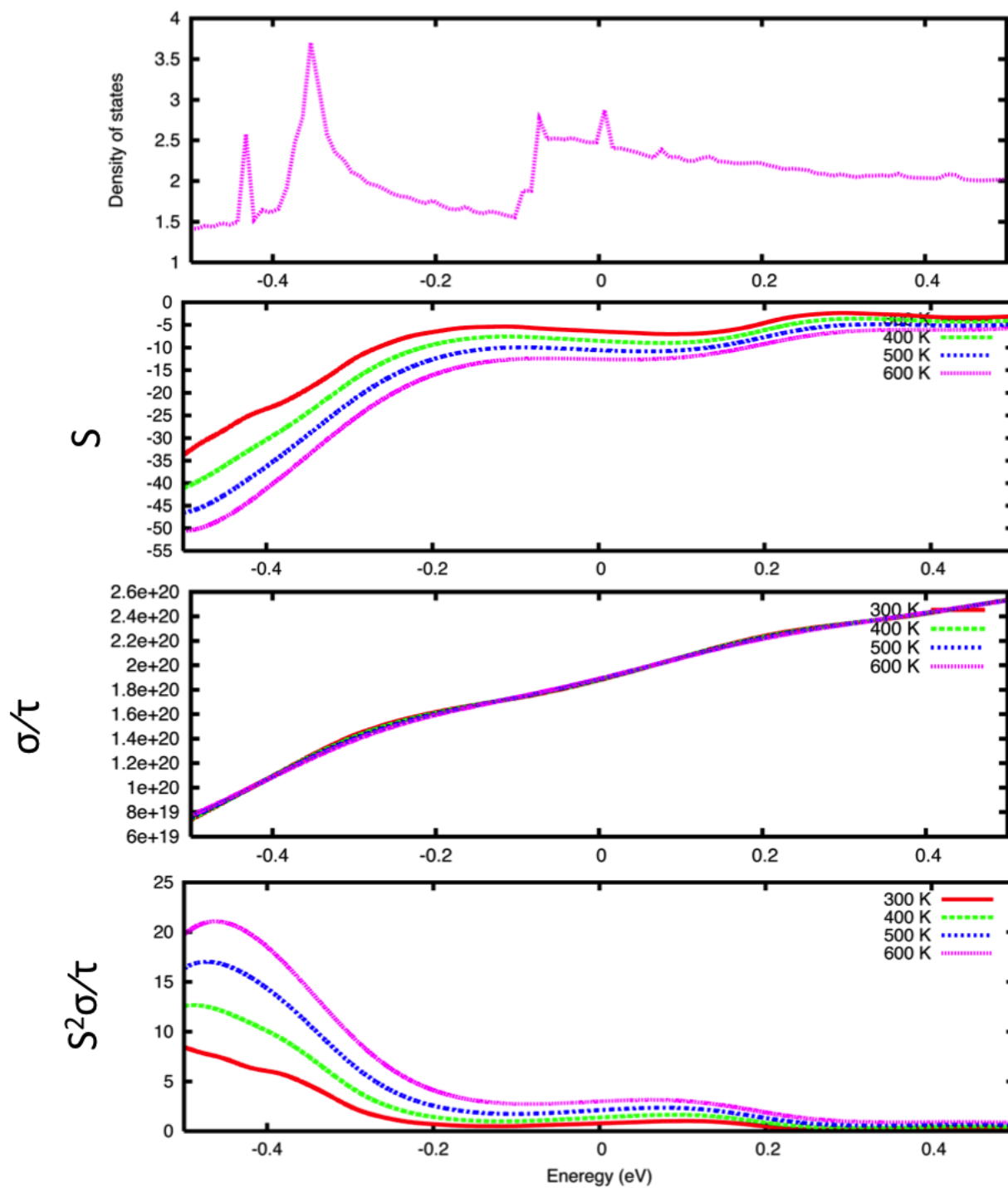
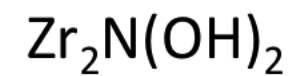
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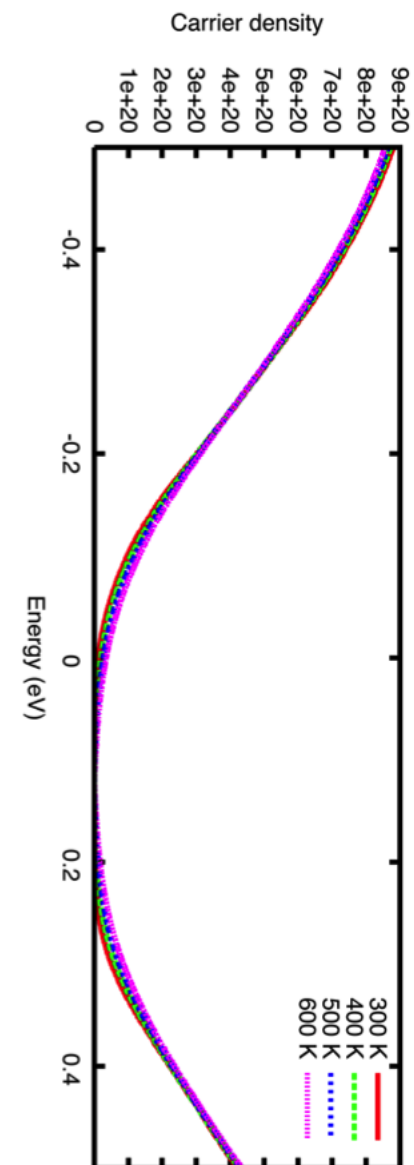
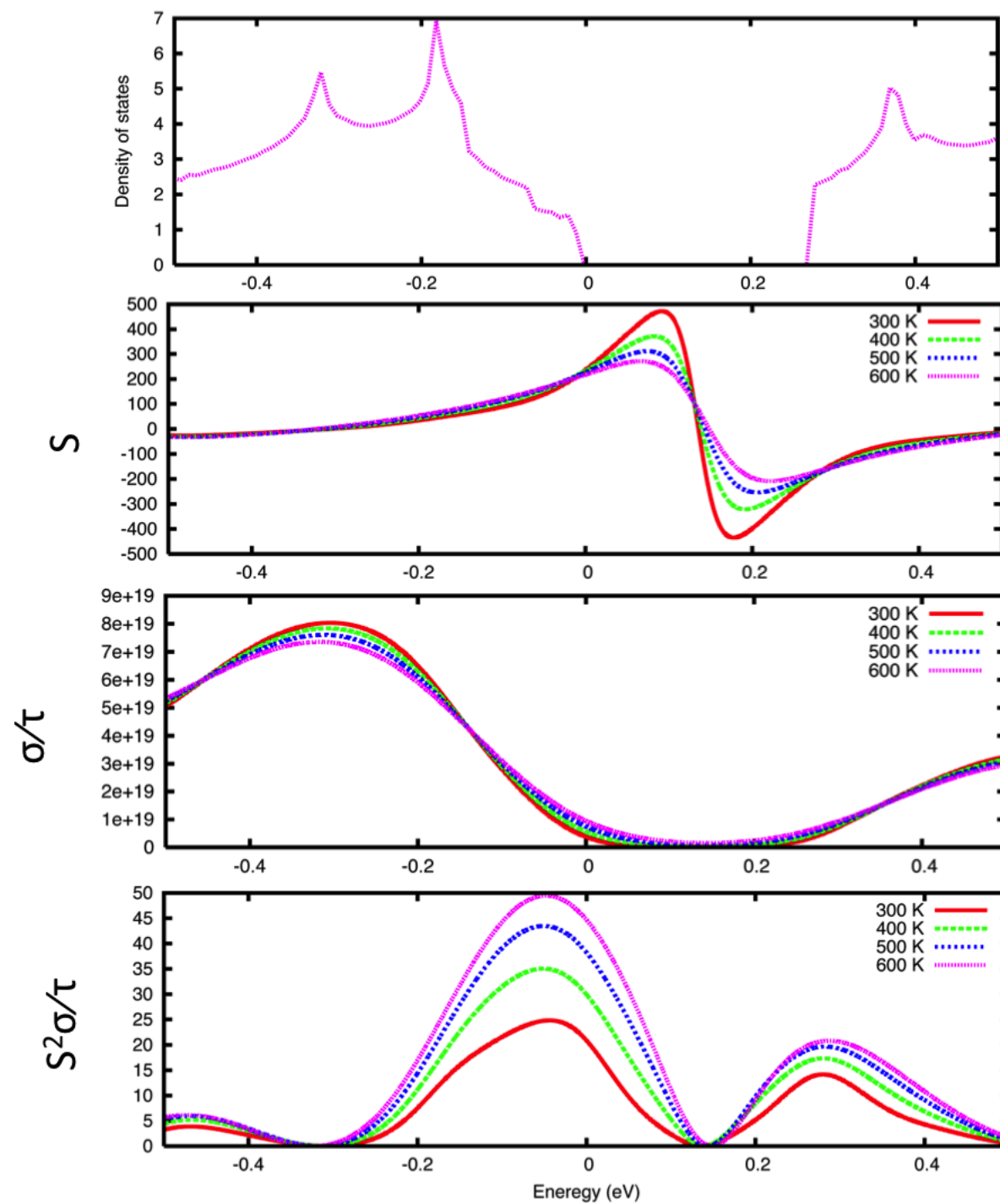
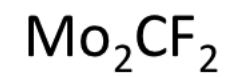


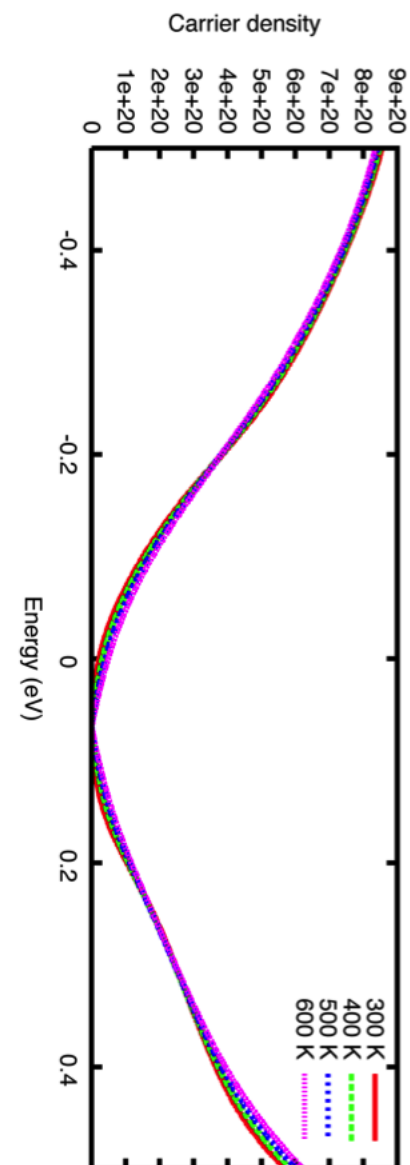
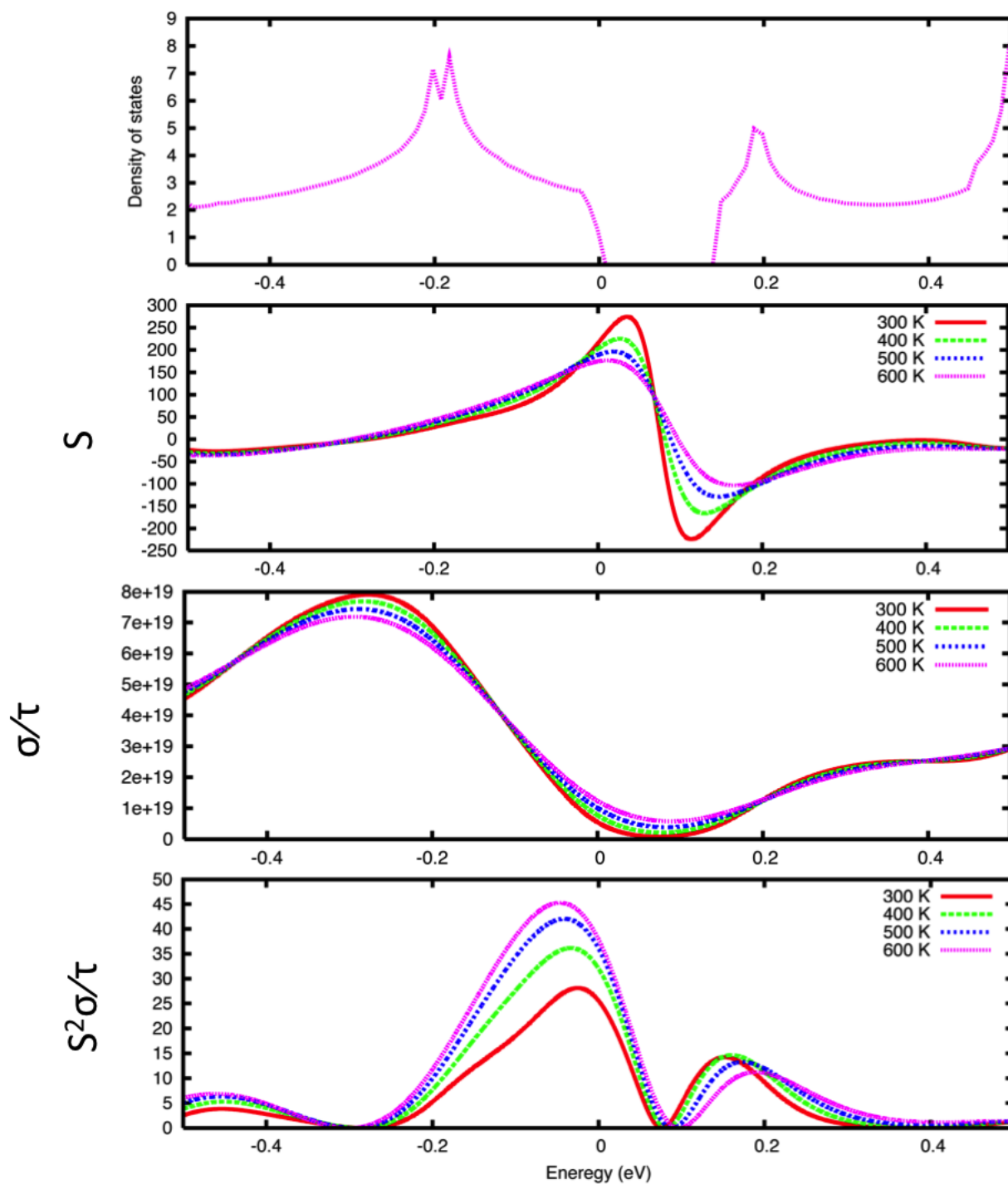
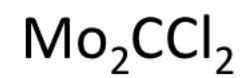


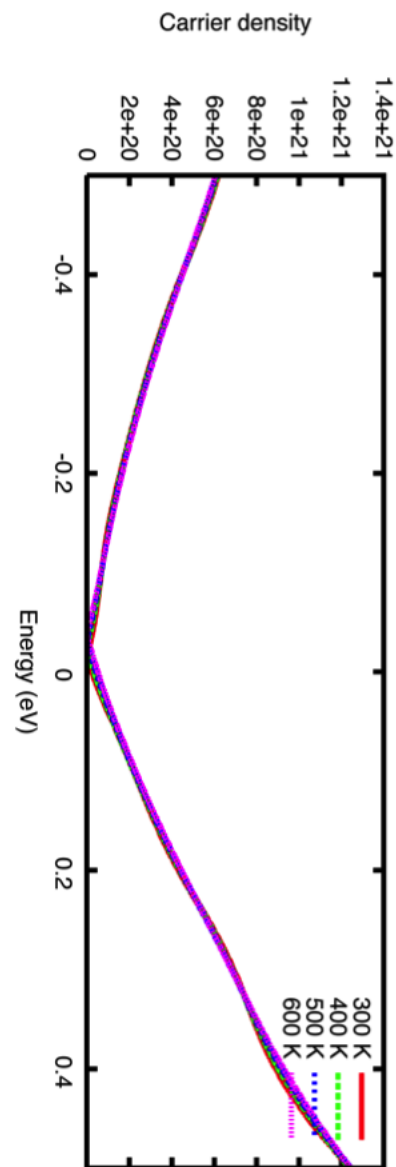
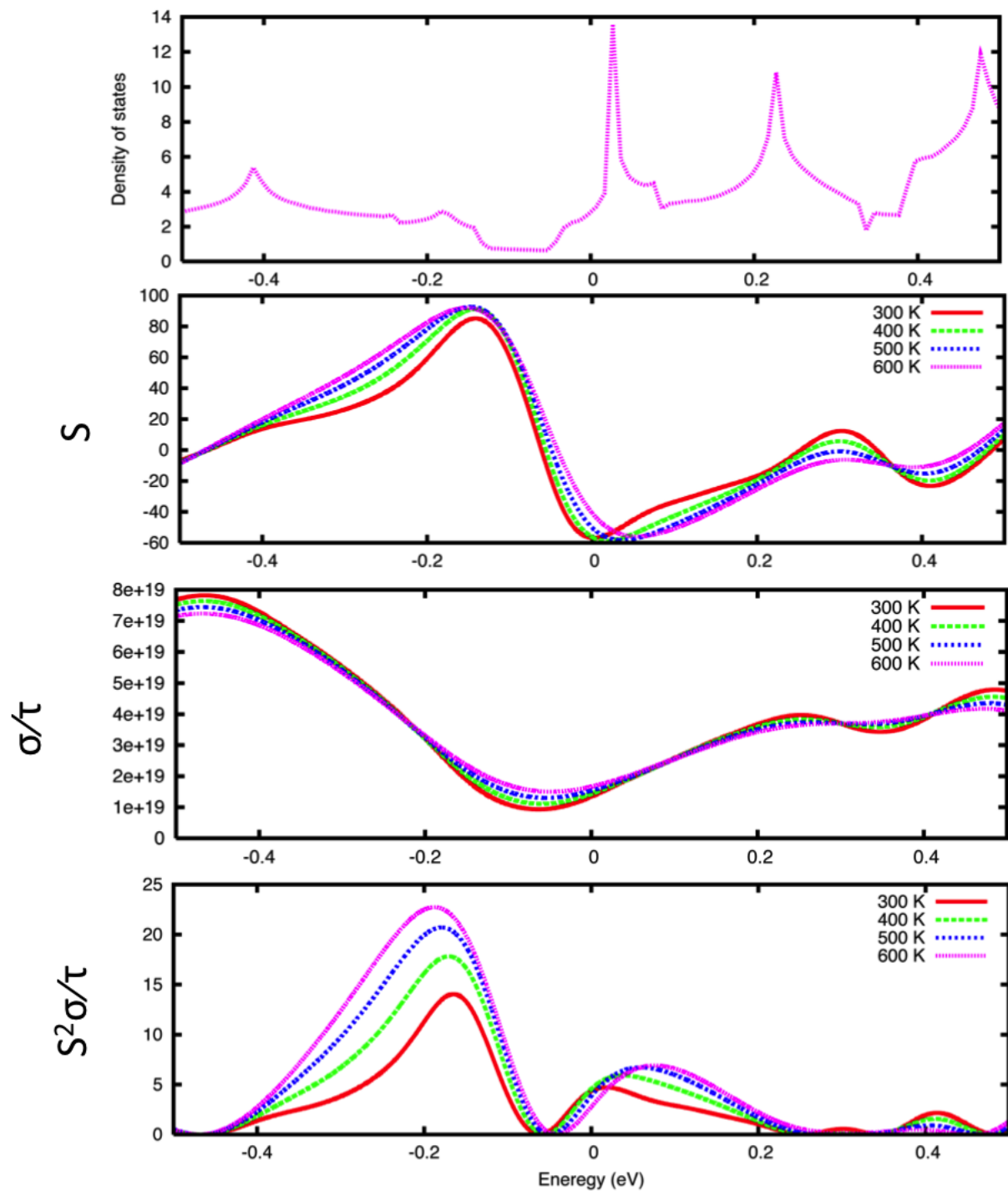
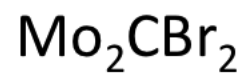
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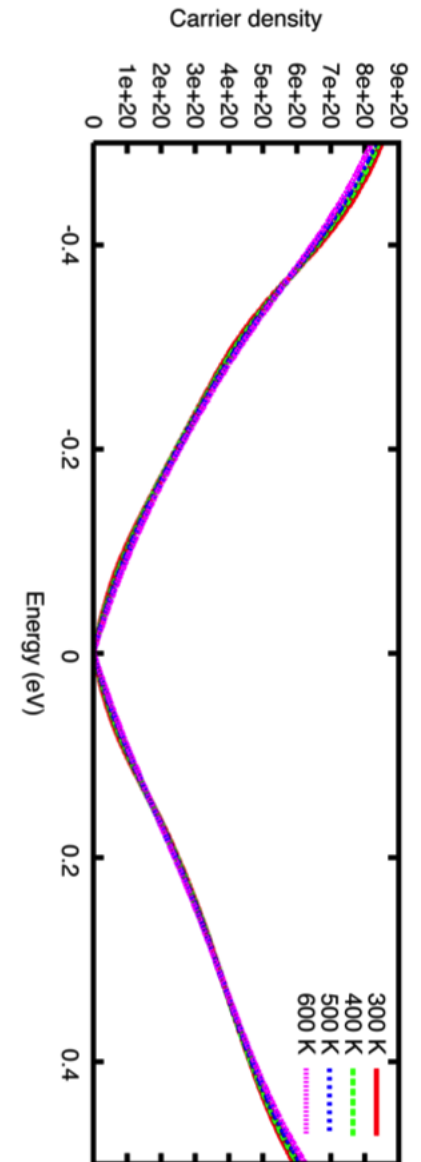
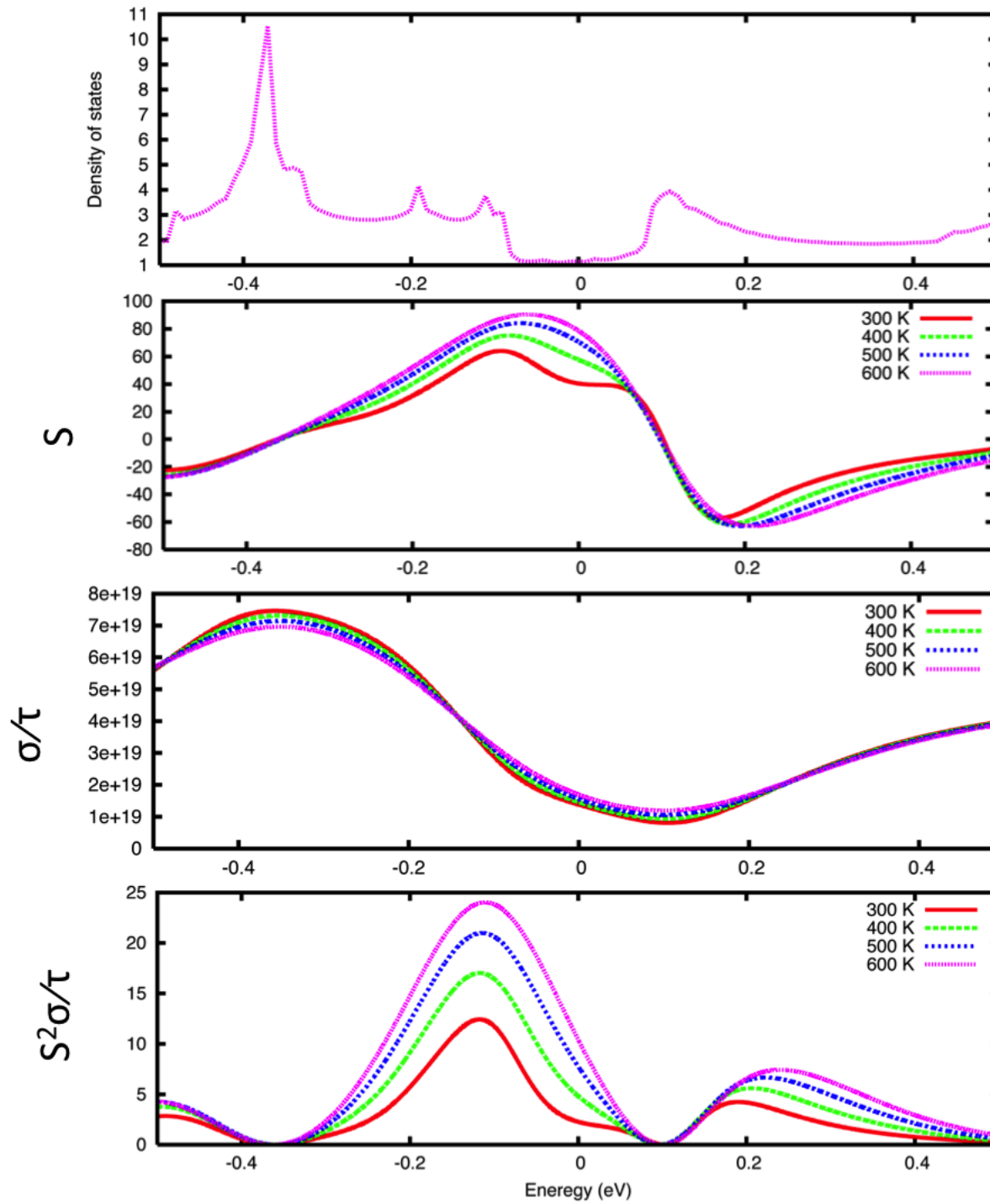
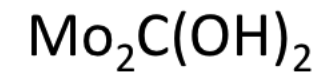


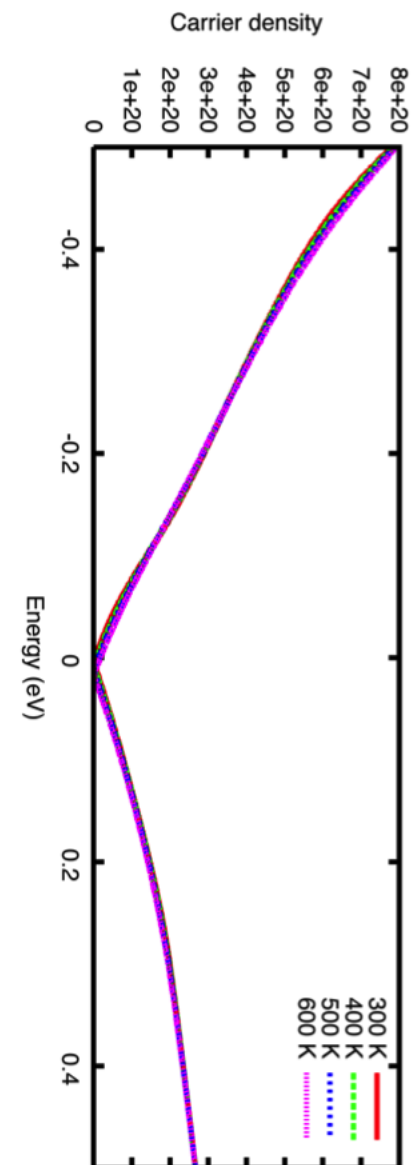
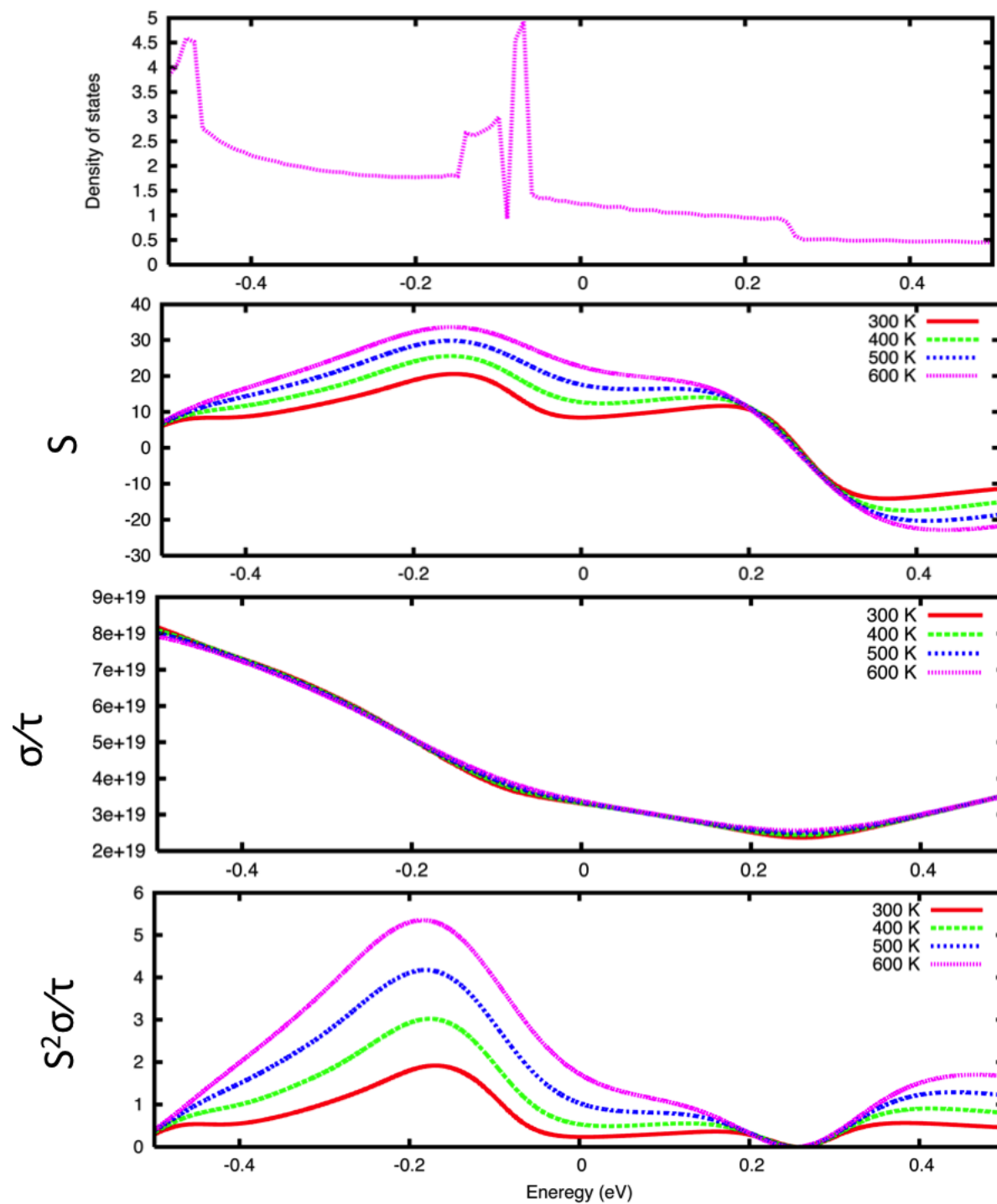
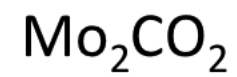


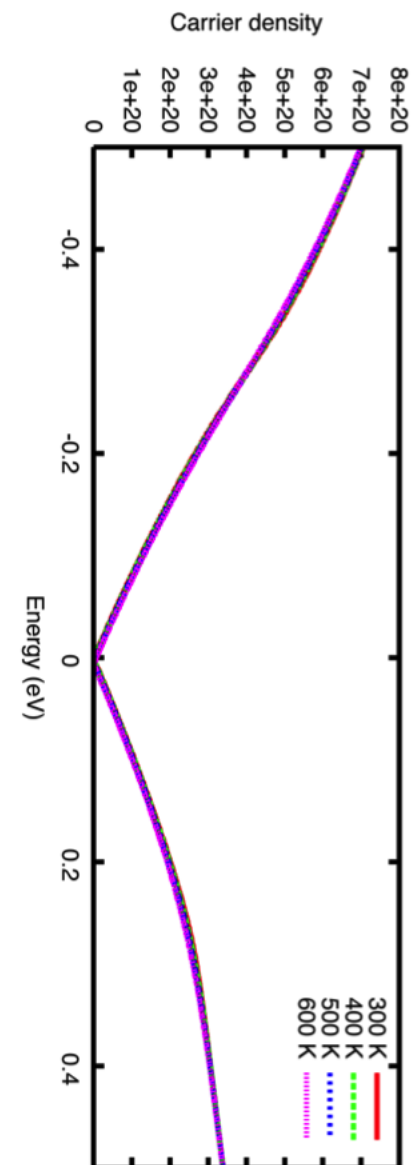
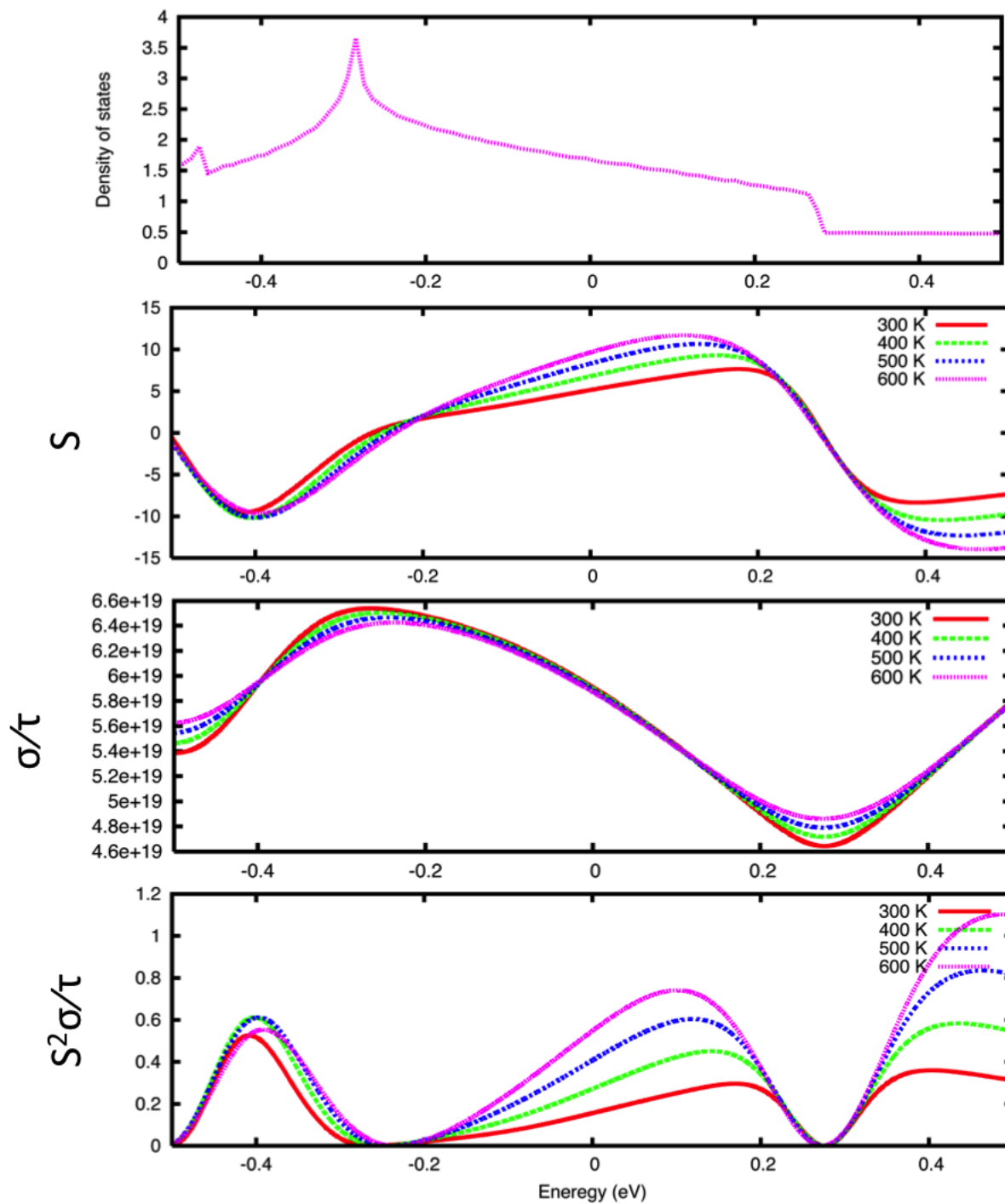
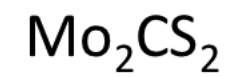


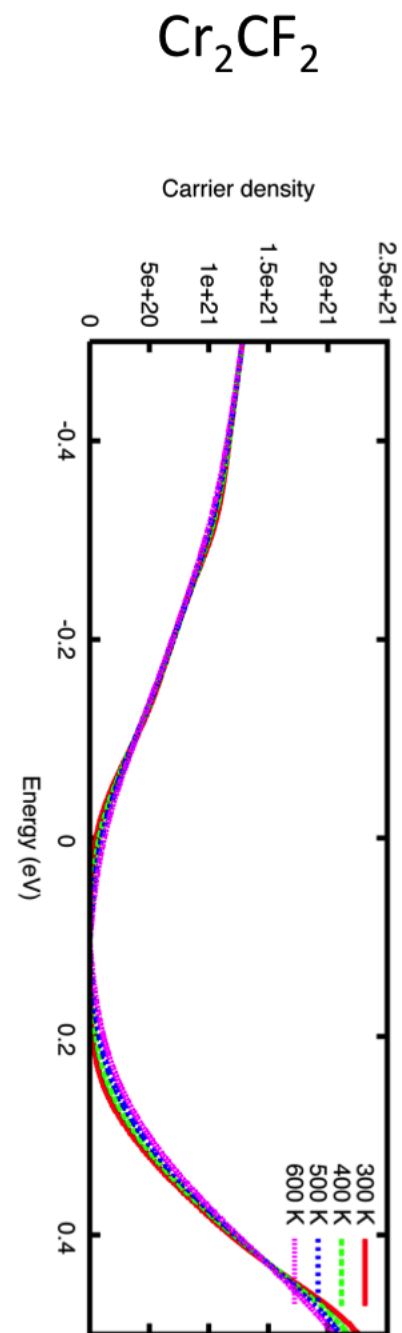
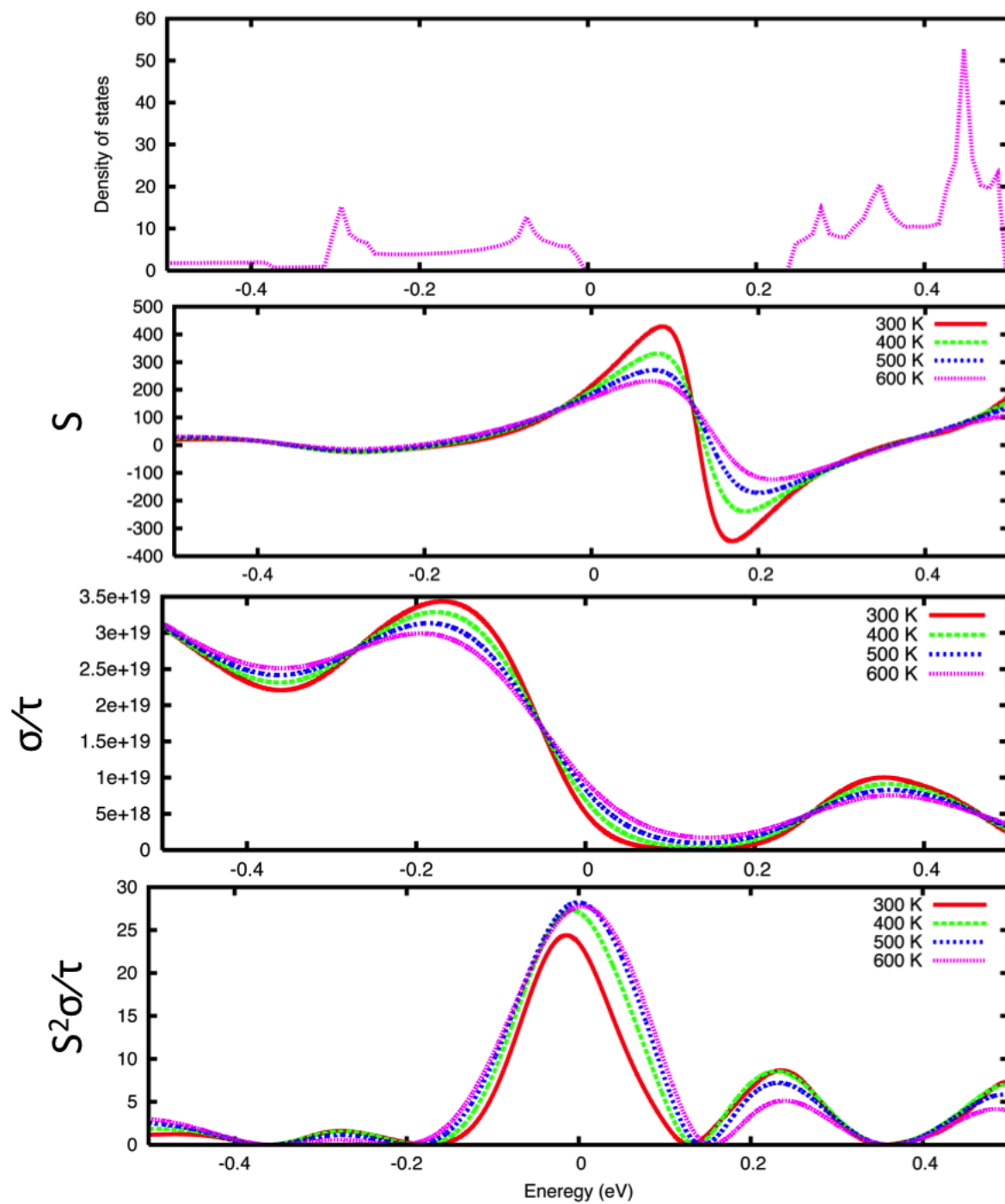


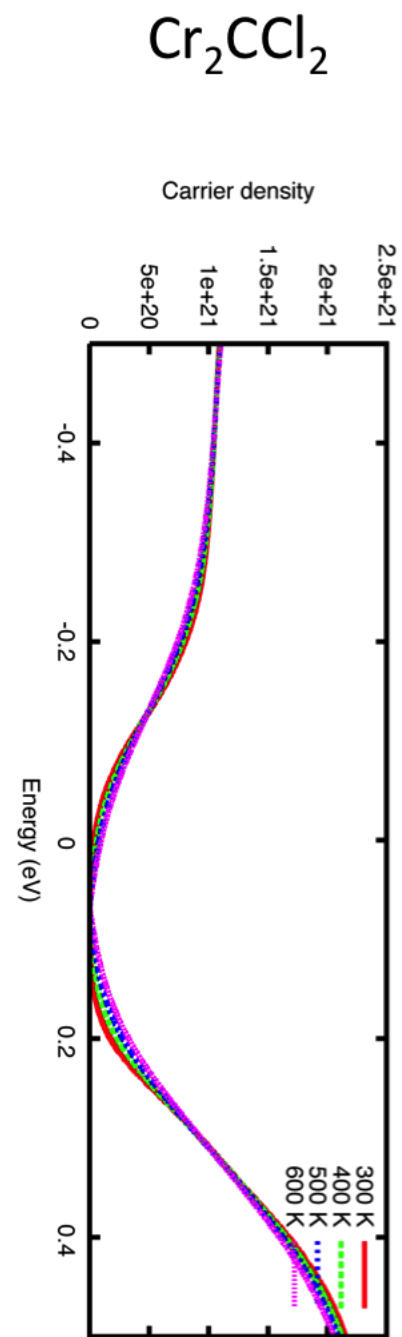
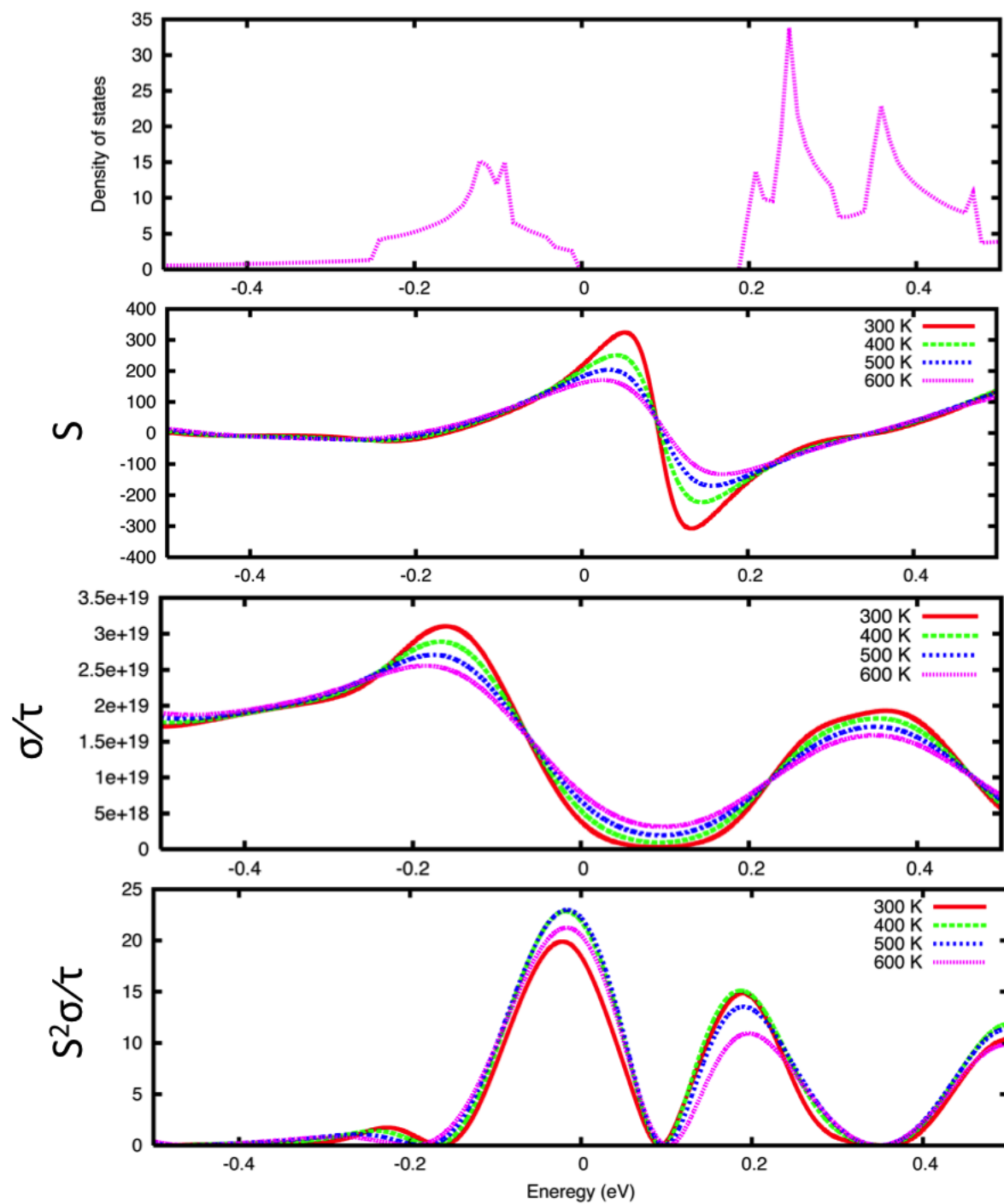


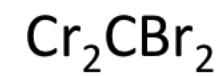






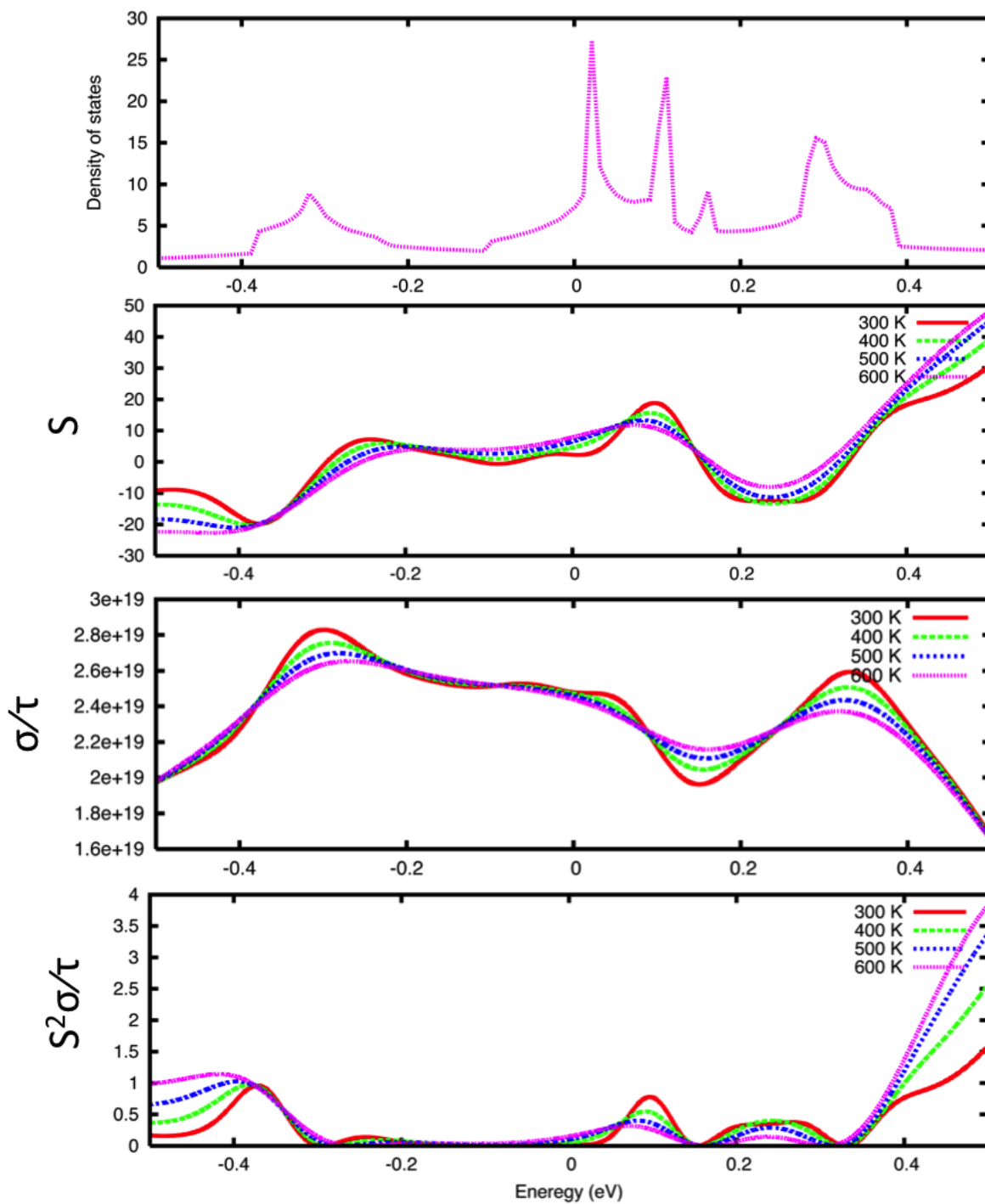
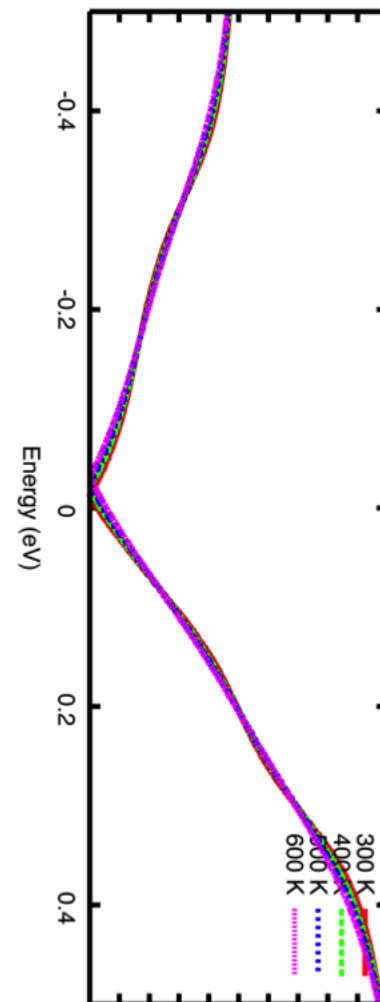


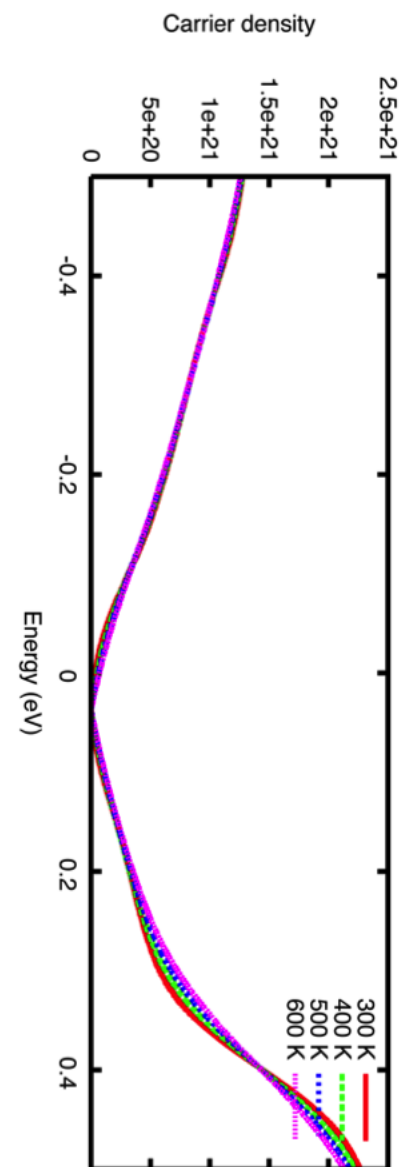
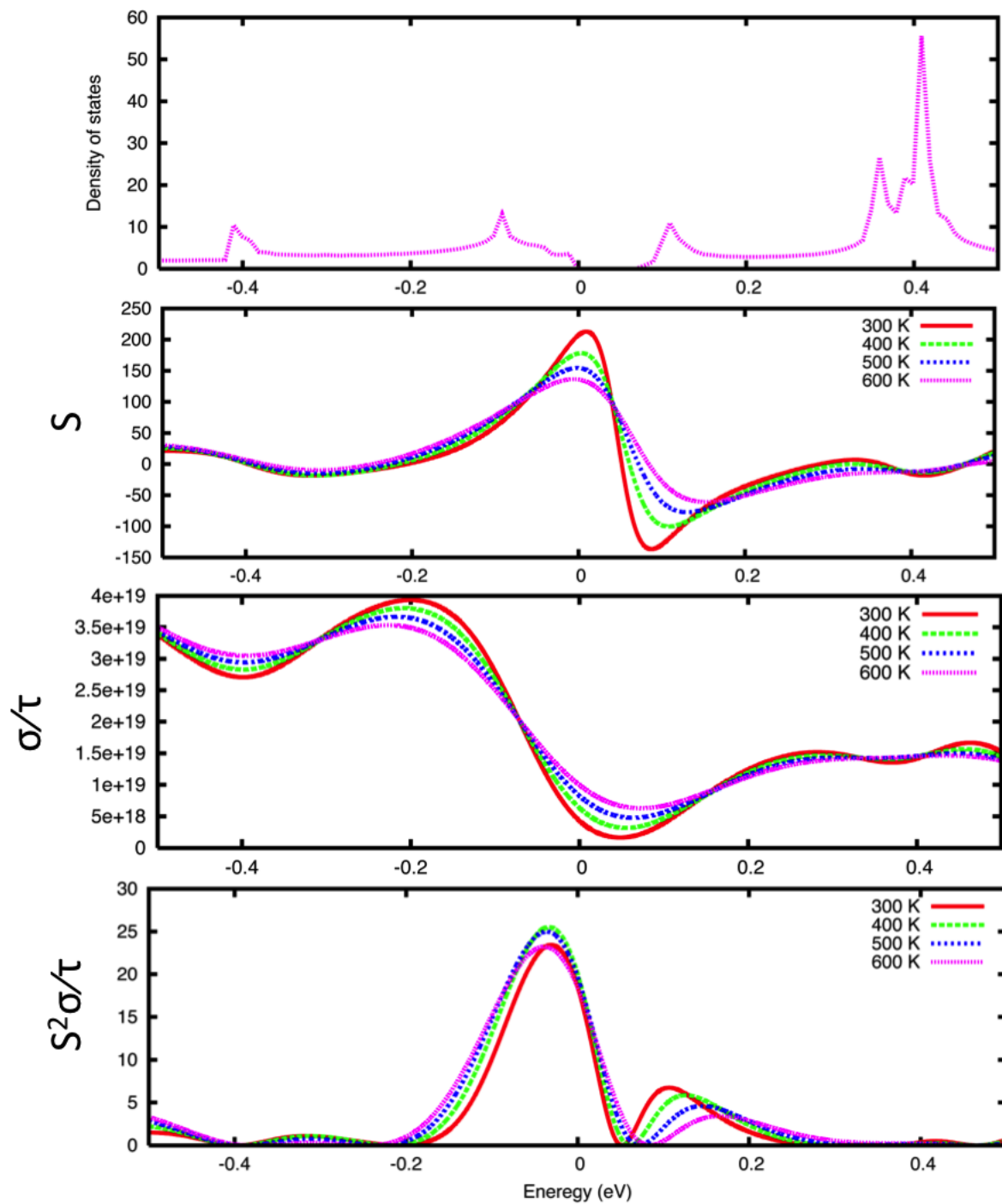
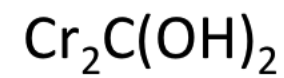


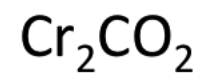


Carrier density

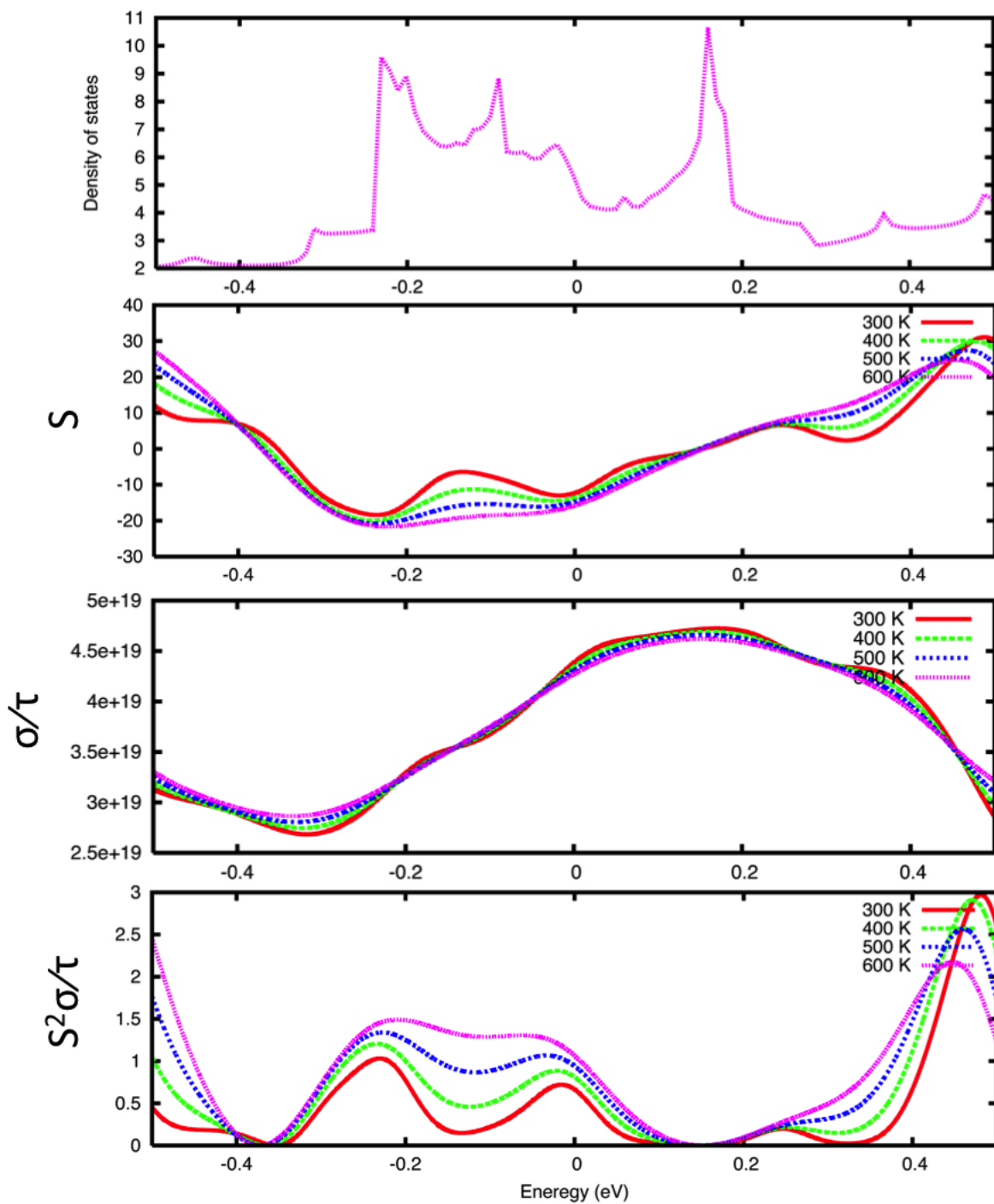
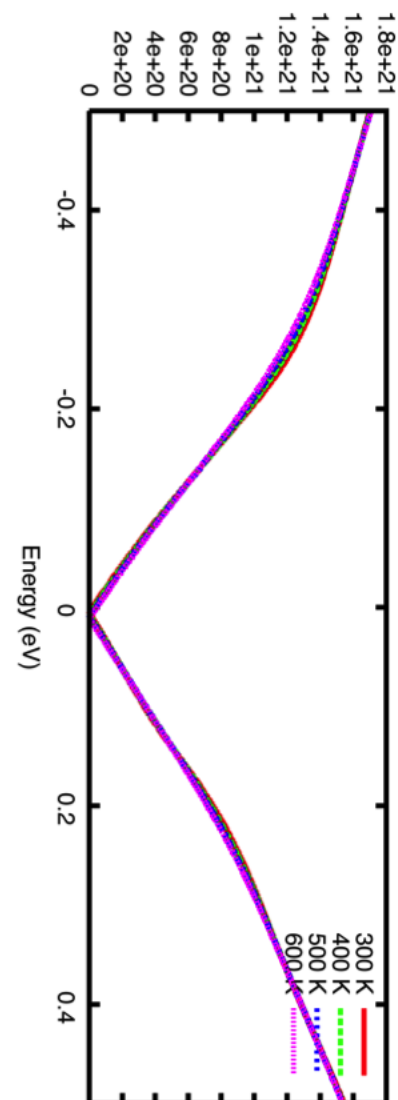
2e+21
1.8e+21
1.6e+21
1.4e+21
1.2e+21
1e+21
8e+20
6e+20
4e+20
2e+20
0

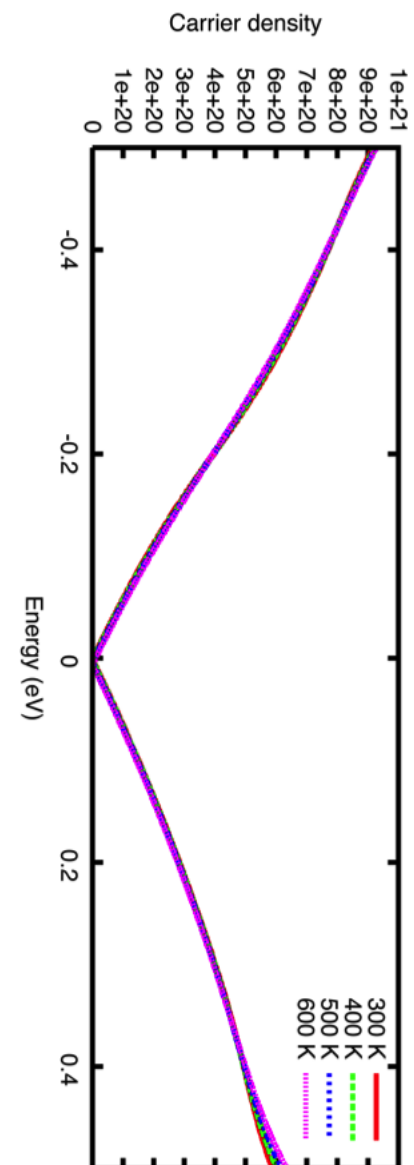
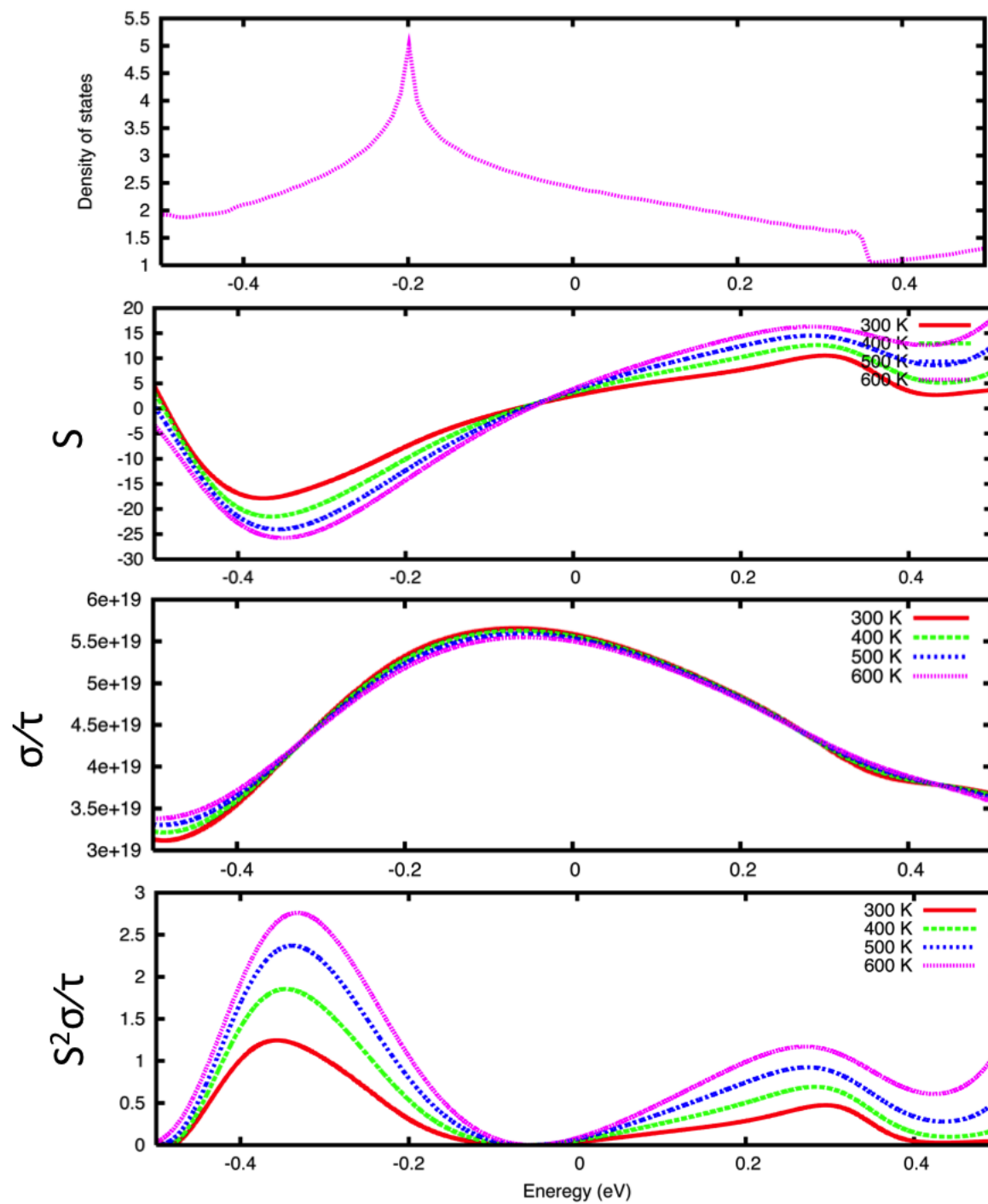
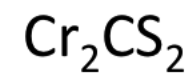




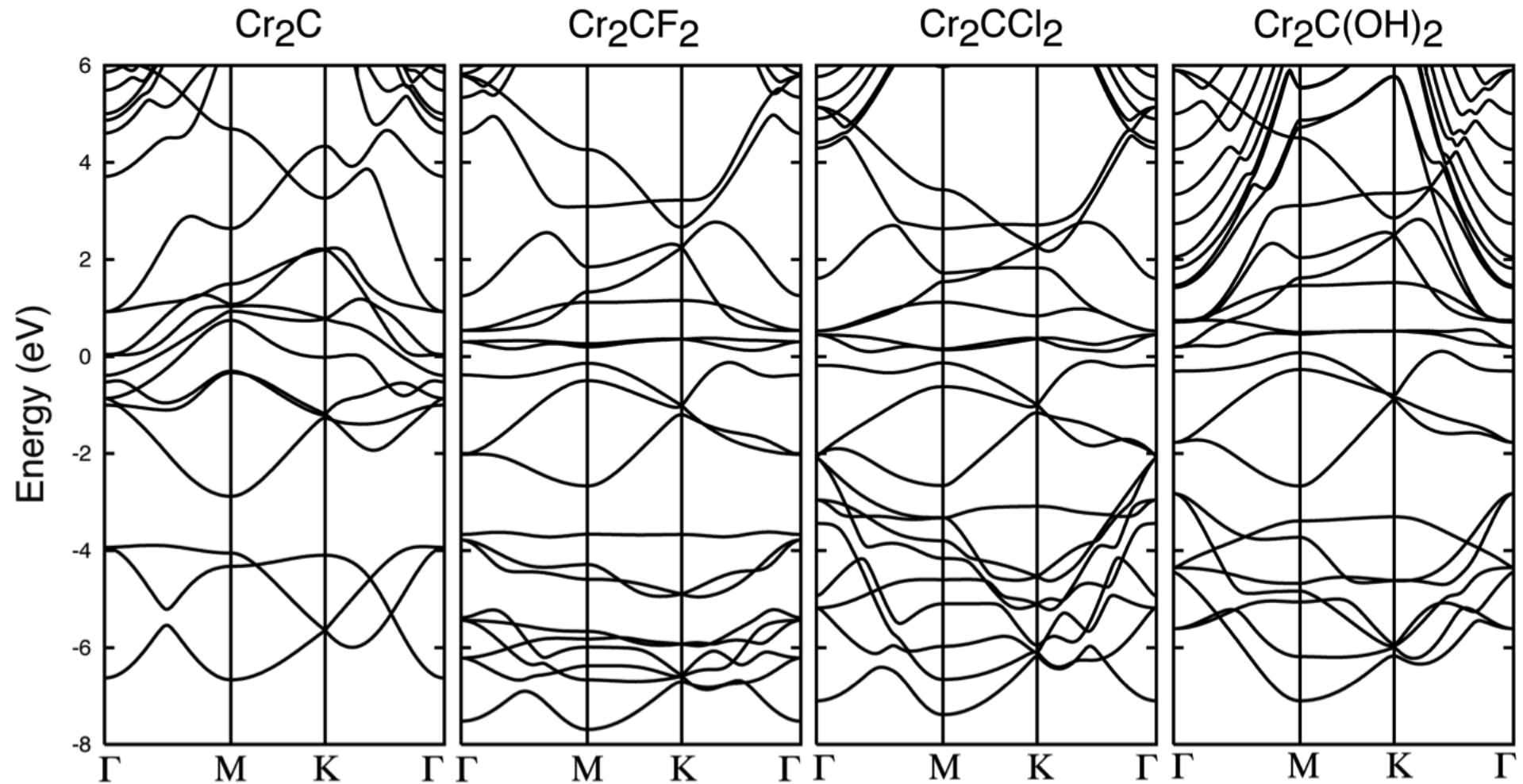


Carrier density

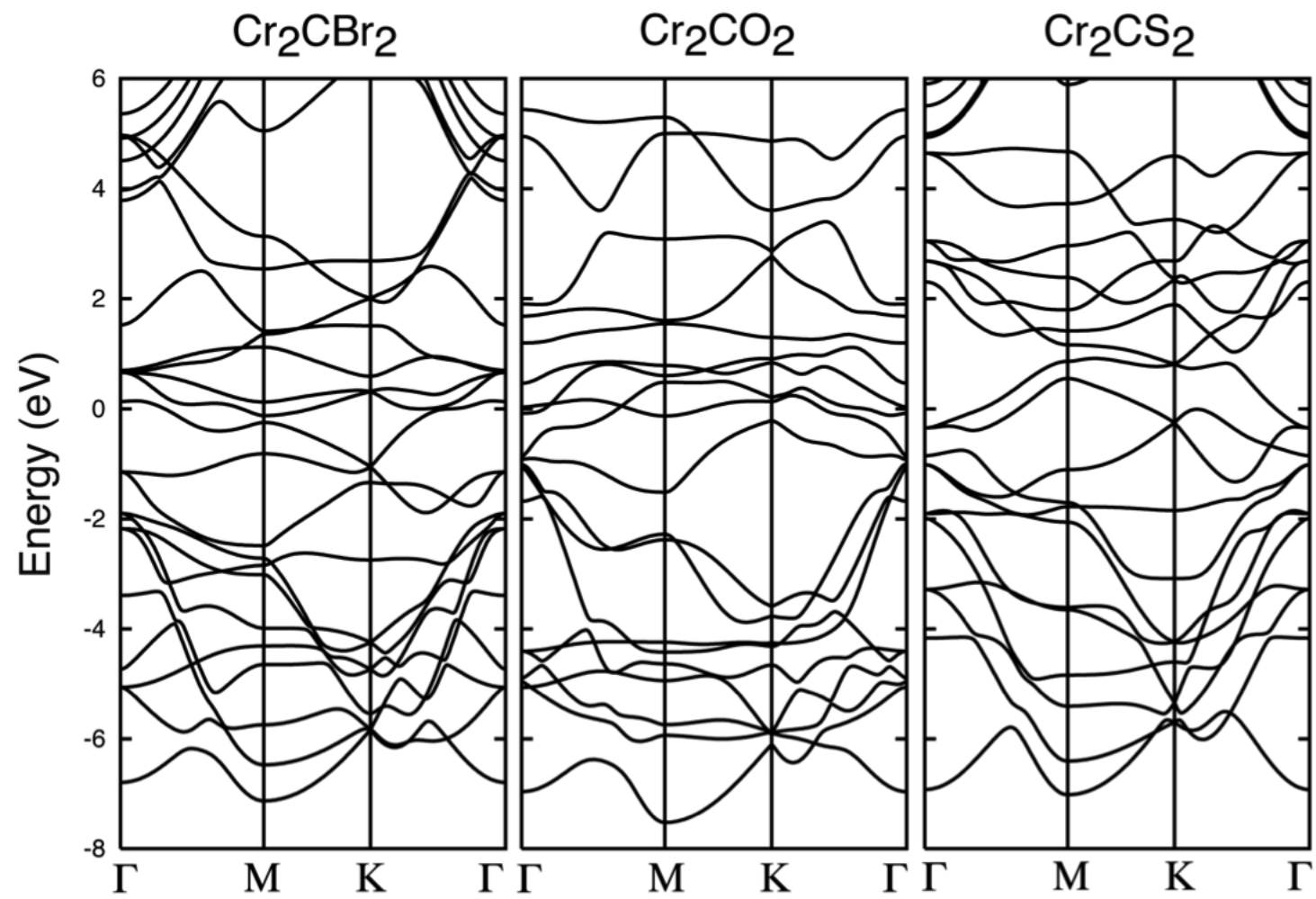




Band structures of pristine and functionalized Cr_2C systems



The energy zero is set to be the top of the highest occupied level.



CIF files of MXene Monolayers

Hf₂CF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.26452
_cell_length_b 3.26466
_cell_length_c 29.88762
_cell_angle_alpha 90.02105
_cell_angle_beta 88.78589
_cell_angle_gamma 120.00611
_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
Hf1 1.0 0.295124 0.642471 0.344890 Biso 1.000000 Hf
Hf2 1.0 0.607974 0.299105 0.424872 Biso 1.000000 Hf
C1 1.0 0.951554 0.970796 0.384882 Biso 1.000000 C
F1 1.0 0.639908 0.314509 0.300128 Biso 1.000000 F
F2 1.0 0.263197 0.626834 0.469632 Biso 1.000000 F

Hf₂CO₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.26502
_cell_length_b      3.26490
_cell_length_c      30.02371
_cell_angle_alpha   86.93873
_cell_angle_beta    95.41159
_cell_angle_gamma   120.00295
_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
  Hf1  1.0  0.396048  0.589204  0.387396  Biso 1.000000  Hf
  Hf2  1.0  0.805554  0.248788  0.479361  Biso 1.000000  Hf
  C1   1.0  0.100798  0.918996  0.433380  Biso 1.000000  C
  O1   1.0  0.703503  0.258214  0.356209  Biso 1.000000  O
  O2   1.0  0.498065  0.579682  0.510546  Biso 1.000000  O
```

Hf₂C(OH)₂-model2

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.27926
_cell_length_b      3.27919
_cell_length_c      30.00652
_cell_angle_alpha   90.90053
_cell_angle_beta    81.23272
_cell_angle_gamma   120.00831
_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
  Hf1  1.0  0.446420  0.689047  0.344768  Biso 1.000000  Hf
  Hf2  1.0  0.636041  0.295556  0.426254  Biso 1.000000  Hf
  C1   1.0  0.041234  0.992309  0.385510  Biso 1.000000  C
  O1   1.0  0.859726  0.389185  0.299428  Biso 1.000000  O
  O2   1.0  0.222720  0.595296  0.471592  Biso 1.000000  O
  H1   1.0  0.917990  0.413621  0.266362  Biso 1.000000  H
  H2   1.0  0.164461  0.570974  0.504662  Biso 1.000000  H
```

Hf₂NF₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.08913
_cell_length_b      3.08922
_cell_length_c      29.95183
_cell_angle_alpha   91.72624
_cell_angle_beta    87.95153
_cell_angle_gamma   120.00038
_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
  Hf1  1.0  0.279069  0.538925  0.402823  Biso 1.000000  Hf
  Hf2  1.0  0.588530  0.220021  0.492990  Biso 1.000000  Hf
  N1   1.0  0.933795  0.879471  0.447908  Biso 1.000000  N
  F1   1.0  0.958373  0.864885  0.355913  Biso 1.000000  F
  F2   1.0  0.909205  0.894053  0.539898  Biso 1.000000  F
```

Hf₂NO₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name          'XCrySDen XSF file'
_cell_length_a           3.21882
_cell_length_b           3.21881
_cell_length_c           29.99438
_cell_angle_alpha        90.02578
_cell_angle_beta         88.81765
_cell_angle_gamma        120.00164
_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
  Hf1  1.0  0.295421  0.642899  0.350044  Biso  1.000000  Hf
  Hf2  1.0  0.606254  0.298687  0.438902  Biso  1.000000  Hf
  N1   1.0  0.950844  0.970795  0.394473  Biso  1.000000  N
  O1   1.0  0.637070  0.313575  0.317313  Biso  1.000000  O
  O2   1.0  0.264621  0.628013  0.471632  Biso  1.000000  O
```

Hf₂N(OH)₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.13074
_cell_length_b      3.12853
_cell_length_c      29.94190
_cell_angle_alpha   83.33437
_cell_angle_beta    90.16907
_cell_angle_gamma   120.02701
_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
  Hf1  1.0  0.345705  0.649218  0.347768  Biso  1.000000  Hf
  Hf2  1.0  0.604139  0.160838  0.437088  Biso  1.000000  Hf
  N1   1.0  0.974923  0.905024  0.392425  Biso  1.000000  N
  O1   1.0  0.041923  0.044183  0.301298  Biso  1.000000  O
  O2   1.0  0.907864  0.765800  0.483557  Biso  1.000000  O
  H1   1.0  0.064723  0.091940  0.268166  Biso  1.000000  H
  H2   1.0  0.885076  0.718174  0.516665  Biso  1.000000  H
```

Nb₂CF₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.22860
_cell_length_b      3.22850
_cell_length_c      30.00088
_cell_angle_alpha   90.01437
_cell_angle_beta    88.82354
_cell_angle_gamma   120.00379
_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
  Nb1  1.0  0.293551  0.642038  0.355116  Biso 1.000000  Nb
  Nb2  1.0  0.608241  0.299542  0.428927  Biso 1.000000  Nb
  C1   1.0  0.950881  0.970780  0.392020  Biso 1.000000  C
  F1   1.0  0.638505  0.314476  0.308966  Biso 1.000000  F
  F2   1.0  0.263380  0.627155  0.475070  Biso 1.000000  F
```


Nb₂CO₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name          'XCrySDen XSF file'
_cell_length_a          3.15390
_cell_length_b          3.15390
_cell_length_c          30.00106
_cell_angle_alpha       90.03550
_cell_angle_beta        88.87267
_cell_angle_gamma       120.00095
_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
Nb1  1.0  0.293557  0.642676  0.368731  Biso 1.000000 Nb
Nb2  1.0  0.606217  0.299536  0.452812  Biso 1.000000 Nb
C1   1.0  0.949879  0.971102  0.410770  Biso 1.000000 C
O1   1.0  0.635759  0.313559  0.332605  Biso 1.000000 O
O2   1.0  0.264031  0.628640  0.488939  Biso 1.000000 O
```

Nb₂C(OH)₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.23100
_cell_length_b      3.23088
_cell_length_c      30.05762
_cell_angle_alpha   90.86558
_cell_angle_beta    81.47973
_cell_angle_gamma   120.00743
_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
  Nb1  1.0  0.428999  0.681511  0.358330  Biso 1.000000  Nb
  Nb2  1.0  0.630463  0.292771  0.433933  Biso 1.000000  Nb
  C1   1.0  0.029727  0.987137  0.396131  Biso 1.000000  C
  O1   1.0  0.843624  0.382290  0.311726  Biso 1.000000  O
  O2   1.0  0.215875  0.592012  0.480538  Biso 1.000000  O
  H1   1.0  0.900956  0.406135  0.278821  Biso 1.000000  H
  H2   1.0  0.158403  0.567973  0.513441  Biso 1.000000  H
```

Sc₂CF₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name          'XCrySDen XSF file'
_cell_length_a          3.28602
_cell_length_b          3.28614
_cell_length_c          29.84225
_cell_angle_alpha       90.01875
_cell_angle_beta        88.77068
_cell_angle_gamma       120.00395
_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
  Sc1  1.0  0.296182  0.642768  0.337928  Biso  1.000000  Sc
  Sc2  1.0  0.607574  0.298610  0.422944  Biso  1.000000  Sc
  C1   1.0  0.951925  0.970707  0.380435  Biso  1.000000  C
  F1   1.0  0.639406  0.314188  0.299581  Biso  1.000000  F
  F2   1.0  0.264476  0.627239  0.461285  Biso  1.000000  F
```

Sc₂CO₂-model3

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.43772
_cell_length_b      3.43771
_cell_length_c      29.75274
_cell_angle_alpha   88.72282
_cell_angle_beta    87.31909
_cell_angle_gamma    120.00268
_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
  Sc1  1.0  0.408925  0.635825  0.304314  Biso  1.000000  Sc
  Sc2  1.0  0.685158  0.257466  0.389724  Biso  1.000000  Sc
  C1   1.0  0.040135  0.941220  0.357339  Biso  1.000000  C
  O1   1.0  0.756602  0.313846  0.282809  Biso  1.000000  O
  O2   1.0  0.002984  0.911954  0.412909  Biso  1.000000  O
```



```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.30789
_cell_length_b      3.30784
_cell_length_c      29.98298
_cell_angle_alpha   90.90748
_cell_angle_beta    81.10091
_cell_angle_gamma   120.00871
_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
  Sc1  1.0  0.457470  0.693922  0.336509  Biso  1.000000  Sc
  Sc2  1.0  0.638864  0.296931  0.422160  Biso  1.000000  Sc
  C1   1.0  0.048169  0.995404  0.379330  Biso  1.000000  C
  O1   1.0  0.865213  0.391801  0.294576  Biso  1.000000  O
  O2   1.0  0.231149  0.598892  0.464084  Biso  1.000000  O
  H1   1.0  0.923477  0.416154  0.261743  Biso  1.000000  H
  H2   1.0  0.173086  0.574879  0.496917  Biso  1.000000  H
```

Ta₂CF₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name          'XCrySDen XSF file'
_cell_length_a          3.20796
_cell_length_b          3.20797
_cell_length_c          30.00093
_cell_angle_alpha       90.02750
_cell_angle_beta        88.82851
_cell_angle_gamma       120.00328
_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
  Ta1  1.0  0.293040  0.641865  0.360927  Biso 1.000000 Ta
  Ta2  1.0  0.608190  0.299733  0.433194  Biso 1.000000 Ta
  C1   1.0  0.950611  0.970800  0.397059  Biso 1.000000 C
  F1   1.0  0.638096  0.314225  0.314406  Biso 1.000000 F
  F2   1.0  0.263261  0.627394  0.479721  Biso 1.000000 F
```

Ta₂CO₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name          'XCrySDen XSF file'
_cell_length_a          3.13153
_cell_length_b          3.13154
_cell_length_c          30.04526
_cell_angle_alpha       90.73315
_cell_angle_beta        84.77940
_cell_angle_gamma       120.00743
_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
Ta1  1.0  0.396825  0.678823  0.362751  Biso 1.000000 Ta
Ta2  1.0  0.640164  0.310627  0.445960  Biso 1.000000 Ta
C1   1.0  0.018500  0.994726  0.404355  Biso 1.000000 C
O1   1.0  0.769328  0.360652  0.326543  Biso 1.000000 O
O2   1.0  0.267618  0.628796  0.482170  Biso 1.000000 O
```

Ta₂C(OH)₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.03014
_cell_length_b      3.03002
_cell_length_c      30.02506
_cell_angle_alpha   83.47543
_cell_angle_beta    90.18668
_cell_angle_gamma   120.00571
_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
Ta1  1.0  0.331075  0.617836  0.372509  Biso 1.000000 Ta
Ta2  1.0  0.601223  0.152216  0.461926  Biso 1.000000 Ta
C1   1.0  0.966127  0.885022  0.417217  Biso 1.000000 C
O1   1.0  0.030706  0.019931  0.326054  Biso 1.000000 O
O2   1.0  0.901701  0.750133  0.508382  Biso 1.000000 O
H1   1.0  0.053950  0.068556  0.293118  Biso 1.000000 H
H2   1.0  0.878106  0.701170  0.541318  Biso 1.000000 H
```


Ti₂CF₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.05874
_cell_length_b      3.05882
_cell_length_c      30.00138
_cell_angle_alpha   90.04304
_cell_angle_beta    88.96212
_cell_angle_gamma   119.99394
_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
  Ti1  1.0  0.291493  0.643070  0.398491  Biso 1.000000 Ti
  Ti2  1.0  0.607196  0.301554  0.474837  Biso 1.000000 Ti
  C1   1.0  0.949349  0.972323  0.436666  Biso 1.000000 C
  F1   1.0  0.634239  0.314154  0.357039  Biso 1.000000 F
  F2   1.0  0.263945  0.630301  0.516289  Biso 1.000000 F
```

Ti₂CO₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.03491
_cell_length_b      3.03482
_cell_length_c      30.00149
_cell_angle_alpha   90.05434
_cell_angle_beta    88.97643
_cell_angle_gamma    119.99948
_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
  Ti1  1.0  0.292609  0.643941  0.399996  Bis  1.000000  Ti
  Ti2  1.0  0.606059  0.301462  0.487187  Bis  1.000000  Ti
  C1   1.0  0.949242  0.972672  0.443593  Bis  1.000000  C
  O1   1.0  0.632927  0.313794  0.369350  Bis  1.000000  O
  O2   1.0  0.265647  0.631597  0.517835  Bis  1.000000  O
```

Ti₂C(OH)₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.07146
_cell_length_b      3.07133
_cell_length_c      30.03318
_cell_angle_alpha   90.76618
_cell_angle_beta    82.26908
_cell_angle_gamma   120.00077
_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
  Ti1  1.0  0.389731  0.663541  0.398738  Biso  1.000000  Ti
  Ti2  1.0  0.593361  0.275489  0.476547  Biso  1.000000  Ti
  C1   1.0  0.991545  0.969510  0.437643  Biso  1.000000  C
  O1   1.0  0.794022  0.360162  0.356151  Biso  1.000000  O
  O2   1.0  0.189014  0.578858  0.519135  Biso  1.000000  O
  H1   1.0  0.848452  0.382778  0.323347  Biso  1.000000  H
  H2   1.0  0.134391  0.556027  0.551941  Biso  1.000000  H
```

Ti₂NF₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.07012
_cell_length_b      3.07037
_cell_length_c      30.01491
_cell_angle_alpha   90.83530
_cell_angle_beta    85.66022
_cell_angle_gamma   119.99641
_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
  Ti1  1.0  0.359762  0.549722  0.368347  Biso  1.000000  Ti
  Ti2  1.0  0.629162  0.194715  0.440097  Biso  1.000000  Ti
  N1   1.0  0.994472  0.872222  0.404219  Biso  1.000000  N
  F1   1.0  0.729978  0.228892  0.326944  Biso  1.000000  F
  F2   1.0  0.258740  0.515449  0.481499  Biso  1.000000  F
```

Ti₂NO₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name          'XCrySDen XSF file'
_cell_length_a          3.02980
_cell_length_b          3.01910
_cell_length_c          29.61518
_cell_angle_alpha       88.04329
_cell_angle_beta        81.73531
_cell_angle_gamma       120.50797
_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
  Ti1  1.0  0.323375  0.621290  0.386023  Biso  1.000000  Ti
  Ti2  1.0  0.483875  0.227631  0.473537  Biso  1.000000  Ti
  N1   1.0  0.903624  0.924400  0.429785  Biso  1.000000  N
  O1   1.0 -0.260361  0.376737  0.353652  Biso  1.000000  O
  O2   1.0  0.067626  0.472164  0.505903  Biso  1.000000  O
```

Ti₂N(OH)₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name          'XCrySDen XSF file'
_cell_length_a          3.06351
_cell_length_b          3.06352
_cell_length_c          30.04061
_cell_angle_alpha       90.74699
_cell_angle_beta        82.31921
_cell_angle_gamma       120.00146
_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
  Ti1  1.0  0.385031  0.661643  0.402557  Biso  1.000000  Ti
  Ti2  1.0  0.594785  0.275984  0.476915  Biso  1.000000  Ti
  N1   1.0  0.989894  0.968806  0.439737  Biso  1.000000  N
  O1   1.0  0.788470  0.357982  0.360377  Biso  1.000000  O
  O2   1.0  0.191350  0.579633  0.519096  Biso  1.000000  O
  H1   1.0  0.842903  0.380784  0.327526  Biso  1.000000  H
  H2   1.0  0.136547  0.556604  0.551946  Biso  1.000000  H
```

V₂CF₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name          'XCrySDen XSF file'
_cell_length_a          2.99034
_cell_length_b          2.99033
_cell_length_c          30.00172
_cell_angle_alpha       90.07376
_cell_angle_beta        89.00786
_cell_angle_gamma       120.00175
_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
V1  1.0  0.290525  0.643706  0.422849  Biso  1.000000  V
V2  1.0  0.608733  0.303635  0.490951  Biso  1.000000  V
C1  1.0  0.949626  0.973671  0.456900  Biso  1.000000  C
F1  1.0  0.633256  0.314492  0.380377  Biso  1.000000  F
F2  1.0  0.265787  0.632801  0.533432  Biso  1.000000  F
```

V₂CO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 2.89425
_cell_length_b 2.90026
_cell_length_c 30.00010
_cell_angle_alpha 85.89667
_cell_angle_beta 94.26115
_cell_angle_gamma 119.93852
_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
V1 1.0 0.300939 0.673771 0.291835 Biso 1.000000 V
V2 1.0 0.653035 0.255110 0.371774 Biso 1.000000 V
C1 1.0 0.976987 0.964431 0.331805 Biso 1.000000 C
O1 1.0 0.604063 0.332601 0.257826 Biso 1.000000 O
O2 1.0 0.349841 0.596169 0.405783 Biso 1.000000 O



```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name          'XCrySDen XSF file'
_cell_length_a          3.00229
_cell_length_b          3.00222
_cell_length_c          30.02407
_cell_angle_alpha       90.71954
_cell_angle_beta        82.63242
_cell_angle_gamma       120.00006
_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
  V1  1.0  0.366854  0.653022  0.422943  Biso  1.000000  V
  V2  1.0  0.587111  0.271874  0.492468  Biso  1.000000  V
  C1  1.0  0.976983  0.962446  0.457704  Biso  1.000000  C
  O1  1.0  0.769672  0.349072  0.380188  Biso  1.000000  O
  O2  1.0  0.184232  0.575798  0.535225  Biso  1.000000  O
  H1  1.0  0.822807  0.371474  0.347403  Biso  1.000000  H
  H2  1.0  0.130917  0.553267  0.568008  Biso  1.000000  H
```

Zr₂CF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.31266
_cell_length_b 3.31193
_cell_length_c 30.00626
_cell_angle_alpha 88.39341
_cell_angle_beta 89.66187
_cell_angle_gamma 120.00432
_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
Zr1 1.0 0.279520 0.627579 0.370367 Biso 1.000000 Zr
Zr2 1.0 0.592908 0.263014 0.452948 Biso 1.000000 Zr
C1 1.0 0.936235 0.945309 0.411653 Biso 1.000000 C
F1 1.0 0.623647 0.310712 0.326432 Biso 1.000000 F
F2 1.0 0.248599 0.579629 0.496889 Biso 1.000000 F

Zr₂CO₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.31913
_cell_length_b      3.31916
_cell_length_c      30.00101
_cell_angle_alpha   94.51791
_cell_angle_beta    87.17352
_cell_angle_gamma   120.00118
_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
  Zr1  1.0  0.483651  0.767176  0.364163  Biso  1.000000  Zr
  Zr2  1.0  0.805723  0.495043  0.457942  Biso  1.000000  Zr
  C1   1.0  0.144687  0.131058  0.411055  Biso  1.000000  C
  O1   1.0  0.820730  0.413547  0.332975  Biso  1.000000  O
  O2   1.0  0.468674  0.848672  0.489135  Biso  1.000000  O
```

Zr₂C(OH)₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.30616
_cell_length_b      3.30618
_cell_length_c      29.86791
_cell_angle_alpha   88.87372
_cell_angle_beta    87.85256
_cell_angle_gamma   120.00600
_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
  Zr1  1.0  0.389223  0.620273  0.334029  Biso  1.000000  Zr
  Zr2  1.0  0.674291  0.247761  0.418683  Biso  1.000000  Zr
  C1   1.0  0.032888  0.934919  0.374441  Biso  1.000000  C
  O1   1.0  0.748561  0.308045  0.288332  Biso  1.000000  O
  O2   1.0  0.981210  0.893008  0.464919  Biso  1.000000  O
  H1   1.0  0.766849  0.323059  0.255645  Biso  1.000000  H
  H2   1.0  0.962453  0.877697  0.497602  Biso  1.000000  H
```

Zr₂NF₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name          'XCrySDen XSF file'
_cell_length_a          3.31225
_cell_length_b          3.31209
_cell_length_c          29.94349
_cell_angle_alpha       90.04229
_cell_angle_beta        88.71966
_cell_angle_gamma       120.10732
_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
  Zr1  1.0  0.296080  0.642529  0.334709  Biso  1.000000  Zr
  Zr2  1.0  0.609325  0.298798  0.412484  Biso  1.000000  Zr
  N1   1.0  0.952721  0.970681  0.373593  Biso  1.000000  N
  F1   1.0  0.641032  0.314763  0.290895  Biso  1.000000  F
  F2   1.0  0.264247  0.626486  0.456304  Biso  1.000000  F
```

Zr₂NO₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.27372
_cell_length_b      3.27344
_cell_length_c      30.00113
_cell_angle_alpha   90.23269
_cell_angle_beta    85.39574
_cell_angle_gamma   120.00967
_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
  Zr1  1.0  0.370368  0.701419  0.358527  Biso  1.000000  Zr
  Zr2  1.0  0.616277  0.328447  0.449418  Biso  1.000000  Zr
  N1   1.0  0.993298  0.014919  0.403973  Biso  1.000000  N
  O1   1.0  0.734845  0.382878  0.325588  Biso  1.000000  O
  O2   1.0  0.251798  0.647004  0.482354  Biso  1.000000  O
```

Zr₂N(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.28294
_cell_length_b 3.28299
_cell_length_c 29.97541
_cell_angle_alpha 90.90323
_cell_angle_beta 81.20797
_cell_angle_gamma 120.00784
_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
Zr1 1.0 0.447784 0.689564 0.343849 Biso 1.000000 Zr
Zr2 1.0 0.635659 0.295274 0.426280 Biso 1.000000 Zr
N1 1.0 0.041705 0.992423 0.385065 Biso 1.000000 N
O1 1.0 0.861188 0.389741 0.298486 Biso 1.000000 O
O2 1.0 0.222258 0.595029 0.471633 Biso 1.000000 O
H1 1.0 0.919560 0.414208 0.265366 Biso 1.000000 H
H2 1.0 0.163889 0.570687 0.504754 Biso 1.000000 H

Mo₂CF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.27772
_cell_length_b 3.27807
_cell_length_c 29.91315
_cell_angle_alpha 90.03268
_cell_angle_beta 88.75828
_cell_angle_gamma 120.02240
_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
Mo1 1.0 0.293435 0.641393 0.349927 Biso 1.000000 Mo
Mo2 1.0 0.610394 0.300048 0.413076 Biso 1.000000 Mo
C1 1.0 0.951974 0.970735 0.381504 Biso 1.000000 C
F1 1.0 0.638174 0.313486 0.306000 Biso 1.000000 F
F2 1.0 0.265684 0.627814 0.457007 Biso 1.000000 F

Mo₂CCl₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.36642
_cell_length_b 3.36654
_cell_length_c 30.00073
_cell_angle_alpha 90.01804
_cell_angle_beta 88.66056
_cell_angle_gamma 120.01123
_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
Mo1 1.0 0.293860 0.640357 0.329637 Biso 1.000000 Mo
Mo2 1.0 0.610237 0.298589 0.391588 Biso 1.000000 Mo
C1 1.0 0.952042 0.969468 0.360612 Biso 1.000000 C
Cl2 1.0 0.643331 0.314966 0.270755 Biso 1.000000 Cl
Cl3 1.0 0.260698 0.623860 0.450473 Biso 1.000000 Cl

Mo₂CBr₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.41936
_cell_length_b 3.41956
_cell_length_c 30.00076
_cell_angle_alpha 90.01839
_cell_angle_beta 88.59299
_cell_angle_gamma 120.01862
_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
Mo1 1.0 0.294287 0.640048 0.319237 Biso 1.000000 Mo
Mo2 1.0 0.610682 0.298018 0.379891 Biso 1.000000 Mo
C1 1.0 0.952481 0.969032 0.349563 Biso 1.000000 C
Br1 1.0 0.645904 0.315880 0.254672 Biso 1.000000 Br
Br2 1.0 0.259115 0.622258 0.444457 Biso 1.000000 Br

Mo₂C(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.30755
_cell_length_b 3.30783
_cell_length_c 30.02127
_cell_angle_alpha 91.37762
_cell_angle_beta 80.86182
_cell_angle_gamma 120.84709
_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
Mo1 1.0 0.434322 0.683379 0.350292 Biso 1.000000 Mo
Mo2 1.0 0.658193 0.298926 0.414306 Biso 1.000000 Mo
C1 1.0 0.046226 0.991128 0.382300 Biso 1.000000 C
O1 1.0 0.845769 0.383027 0.306015 Biso 1.000000 O
O2 1.0 0.246757 0.599337 0.458580 Biso 1.000000 O
H1 1.0 0.906190 0.405299 0.273076 Biso 1.000000 H
H2 1.0 0.186199 0.576877 0.491524 Biso 1.000000 H

Mo₂CO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 2.88362
_cell_length_b 2.88369
_cell_length_c 30.00078
_cell_angle_alpha 91.38995
_cell_angle_beta 88.32800
_cell_angle_gamma 120.00671
_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
Mo1 1.0 0.276756 0.538964 0.467152 Biso 1.000000 Mo
Mo2 1.0 0.588417 0.217909 0.559034 Biso 1.000000 Mo
C1 1.0 0.932581 0.878438 0.513092 Biso 1.000000 C
O1 1.0 0.953156 0.866815 0.426253 Biso 1.000000 O
O2 1.0 0.912045 0.890046 0.599930 Biso 1.000000 O

Mo₂CS₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.07984
_cell_length_b 3.07984
_cell_length_c 26.30474
_cell_angle_alpha 91.69219
_cell_angle_beta 87.96307
_cell_angle_gamma 119.99981
_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
Mo1 1.0 0.277631 0.538484 0.463641 Biso 1.000000 Mo
Mo2 1.0 0.587552 0.218383 0.562543 Biso 1.000000 Mo
C1 1.0 0.932592 0.878432 0.513092 Biso 1.000000 C
S1 1.0 0.958859 0.863582 0.402088 Biso 1.000000 S
S2 1.0 0.906321 0.893292 0.624096 Biso 1.000000 S

Cr₂CF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.02569
_cell_length_b 3.02571
_cell_length_c 30.00362
_cell_angle_alpha 90.09004
_cell_angle_beta 88.95126
_cell_angle_gamma 119.99998
_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
Cr1 1.0 0.289867 0.642473 0.416044 Biso 1.000000 Cr
Cr2 1.0 0.609207 0.303065 0.476466 Biso 1.000000 Cr
C1 1.0 0.949493 0.972762 0.446255 Biso 1.000000 C
F1 1.0 0.632581 0.313251 0.374779 Biso 1.000000 F
F2 1.0 0.266039 0.632274 0.517734 Biso 1.000000 F

Cr₂CCl₂₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.16116
_cell_length_b 3.16113
_cell_length_c 29.99261
_cell_angle_alpha 90.06485
_cell_angle_beta 88.80658
_cell_angle_gamma 120.00035
_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
Cr1 1.0 0.288990 0.639521 0.379875 Biso 1.000000 Cr
Cr2 1.0 0.607379 0.299333 0.438153 Biso 1.000000 Cr
C1 1.0 0.948185 0.969430 0.409012 Biso 1.000000 C
Cl2 1.0 0.636439 0.312673 0.324752 Biso 1.000000 Cl
Cl3 1.0 0.259913 0.626198 0.493275 Biso 1.000000 Cl
Cr₂CCl₂

Cr₂CBr₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.25593
_cell_length_b 3.25595
_cell_length_c 30.00083
_cell_angle_alpha 90.04881
_cell_angle_beta 88.71431
_cell_angle_gamma 120.00055
_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
Cr1 1.0 0.289488 0.638456 0.358071 Biso 1.000000 Cr
Cr2 1.0 0.608040 0.298157 0.412844 Biso 1.000000 Cr
C1 1.0 0.948724 0.968307 0.385457 Biso 1.000000 C
Br1 1.0 0.639261 0.312847 0.297376 Biso 1.000000 Br
Br2 1.0 0.258301 0.623742 0.473538 Biso 1.000000 Br

Cr₂C(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.04459
_cell_length_b 3.04463
_cell_length_c 30.02934
_cell_angle_alpha 90.74664
_cell_angle_beta 82.41885
_cell_angle_gamma 120.00452
_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
Cr1 1.0 0.369523 0.654704 0.414586 Biso 1.000000 Cr
Cr2 1.0 0.601721 0.278666 0.475939 Biso 1.000000 Cr
C1 1.0 0.985618 0.966678 0.445266 Biso 1.000000 C
O1 1.0 0.771258 0.350285 0.373091 Biso 1.000000 O
O2 1.0 0.199906 0.583100 0.517436 Biso 1.000000 O
H1 1.0 0.825432 0.373066 0.340309 Biso 1.000000 H
H2 1.0 0.145710 0.560125 0.550219 Biso 1.000000 H

Cr₂CO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 2.78211
_cell_length_b 2.81116
_cell_length_c 30.00302
_cell_angle_alpha 90.01852
_cell_angle_beta 86.96729
_cell_angle_gamma 120.34563
_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
Cr1 1.0 0.261106 0.634806 0.483358 Biso 1.000000 Cr
Cr2 1.0 0.644521 0.326809 0.566816 Biso 1.000000 Cr
C1 1.0 0.952791 0.980808 0.525091 Biso 1.000000 C
O1 1.0 0.638588 0.323491 0.448520 Biso 1.000000 O
O2 1.0 0.267014 0.638124 0.601648 Biso 1.000000 O

Cr₂CS₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 2.93220
_cell_length_b 2.93219
_cell_length_c 29.99313
_cell_angle_alpha 91.42879
_cell_angle_beta 88.31092
_cell_angle_gamma 120.00050
_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
Cr1 1.0 0.278154 0.537735 0.457648 Biso 1.000000 Cr
Cr2 1.0 0.593534 0.215194 0.535047 Biso 1.000000 Cr
C1 1.0 0.935838 0.876466 0.496348 Biso 1.000000 C
S1 1.0 0.956638 0.863984 0.406666 Biso 1.000000 S
S2 1.0 0.915044 0.888960 0.586033 Biso 1.000000 S

CIF files of considered MXene Multilayers layers



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CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 5.33437
_cell_length_b 3.08123
_cell_length_c 11.40351
_cell_angle_alpha 90
_cell_angle_beta 132.77565
_cell_angle_gamma 90
_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
Hf1 1.0 0.432914 0.500000 0.338652 Biso 1.000000 Hf
Hf2 1.0 0.567086 0.500000 0.661348 Biso 1.000000 Hf
Hf3 1.0 0.932914 0.000000 0.338652 Biso 1.000000 Hf
Hf4 1.0 0.067086 0.000000 0.661348 Biso 1.000000 Hf
N1 1.0 0.500000 0.000000 0.500000 Biso 1.000000 N
N2 1.0 -0.000000 0.500000 0.500000 Biso 1.000000 N
F1 1.0 0.021325 0.000000 0.170488 Biso 1.000000 F
F2 1.0 0.978674 0.000000 0.829512 Biso 1.000000 F
F3 1.0 0.521325 0.500000 0.170488 Biso 1.000000 F
F4 1.0 0.478674 0.500000 0.829512 Biso 1.000000 F

Hf₂CO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.27348
_cell_length_b 3.27348
_cell_length_c 7.17532
_cell_angle_alpha 89.99911
_cell_angle_beta 90.00086
_cell_angle_gamma 120.00289
_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
Hf1 1.0 0.333340 0.666660 0.308592 Biso 1.000000 Hf
Hf2 1.0 0.666660 0.333340 0.691408 Biso 1.000000 Hf
C1 1.0 -0.000000 0.000000 0.500000 Biso 1.000000 C
O1 1.0 0.666659 0.333342 0.180154 Biso 1.000000 O
O2 1.0 0.333341 0.666658 0.819846 Biso 1.000000 O

Hf₂C(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name	'XCrySDen XSF file'				
_cell_length_a	3.26798				
_cell_length_b	3.26798				
_cell_length_c	8.79767				
_cell_angle_alpha	89.99580				
_cell_angle_beta	90.00420				
_cell_angle_gamma	120.00143				
_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					
Hf1	1.0	0.666697	0.333303	0.638501	Biso 1.000000 Hf
Hf2	1.0	0.333303	0.666697	0.361499	Biso 1.000000 Hf
C1	1.0	0.000000	0.000000	0.500000	Biso 1.000000 C
O1	1.0	0.666645	0.333355	0.213488	Biso 1.000000 O
O2	1.0	0.333355	0.666645	0.786512	Biso 1.000000 O
H1	1.0	0.666657	0.333342	0.101109	Biso 1.000000 H
H2	1.0	0.333344	0.666658	0.898891	Biso 1.000000 H

Hf₂NF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 5.33437
_cell_length_b 3.08123
_cell_length_c 11.40351
_cell_angle_alpha 90
_cell_angle_beta 132.77565
_cell_angle_gamma 90
_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
Hf1 1.0 0.432914 0.500000 0.338652 Biso 1.000000 Hf
Hf2 1.0 0.567086 0.500000 0.661348 Biso 1.000000 Hf
Hf3 1.0 0.932914 0.000000 0.338652 Biso 1.000000 Hf
Hf4 1.0 0.067086 0.000000 0.661348 Biso 1.000000 Hf
N1 1.0 0.500000 0.000000 0.500000 Biso 1.000000 N
N2 1.0 -0.000000 0.500000 0.500000 Biso 1.000000 N
F1 1.0 0.021325 0.000000 0.170488 Biso 1.000000 F
F2 1.0 0.978674 0.000000 0.829512 Biso 1.000000 F
F3 1.0 0.521325 0.500000 0.170488 Biso 1.000000 F
F4 1.0 0.478674 0.500000 0.829512 Biso 1.000000 F

Hf₂NO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.22584
_cell_length_b 3.22584
_cell_length_c 7.20681
_cell_angle_alpha 89.99945
_cell_angle_beta 90.00056
_cell_angle_gamma 120.00383
_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
Hf1 1.0 0.333350 0.666650 0.315284 Biso 1.000000 Hf
Hf2 1.0 0.666650 0.333350 0.684716 Biso 1.000000 Hf
N1 1.0 0.000000 -0.000000 0.500000 Biso 1.000000 N
O1 1.0 0.666652 0.333347 0.180290 Biso 1.000000 O
O2 1.0 0.333348 0.666653 0.819710 Biso 1.000000 O

Hf₂N(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 5.44181
_cell_length_b 3.14040
_cell_length_c 9.08292
_cell_angle_alpha 90
_cell_angle_beta 101.38667
_cell_angle_gamma 90
_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
Hf1 1.0 0.715834 0.000000 0.146612 Biso 1.000000 Hf
Hf2 1.0 0.284166 0.000000 0.853388 Biso 1.000000 Hf
Hf3 1.0 0.215833 0.500000 0.146611 Biso 1.000000 Hf
Hf4 1.0 0.784166 0.500000 0.853387 Biso 1.000000 Hf
N1 1.0 0.500000 0.500000 -0.000000 Biso 1.000000 N
N2 1.0 -0.000000 0.000000 -0.000000 Biso 1.000000 N
O1 1.0 0.098737 0.000000 0.297826 Biso 1.000000 O
O2 1.0 0.901262 0.000000 0.702175 Biso 1.000000 O
O3 1.0 0.598740 0.500000 0.297829 Biso 1.000000 O
O4 1.0 0.401261 0.500000 0.702172 Biso 1.000000 O
H1 1.0 0.136013 0.000000 0.409314 Biso 1.000000 H
H2 1.0 0.863987 0.000000 0.590686 Biso 1.000000 H
H3 1.0 0.636012 0.500000 0.409312 Biso 1.000000 H
H4 1.0 0.363989 0.500000 0.590688 Biso 1.000000 H

Nb₂CF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.23010
_cell_length_b 3.23010
_cell_length_c 7.50390
_cell_angle_alpha 89.99950
_cell_angle_beta 90.00048
_cell_angle_gamma 120.00188
_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
Nb1 1.0 0.333333 0.666667 0.352662 Biso 1.000000 Nb
Nb2 1.0 0.666667 0.333333 0.647345 Biso 1.000000 Nb
C1 1.0 -0.000000 -0.000000 0.500006 Biso 1.000000 C
F1 1.0 0.666661 0.333339 0.168817 Biso 1.000000 F
F2 1.0 0.333339 0.666661 0.831170 Biso 1.000000 F

Nb₂CO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.15553
_cell_length_b 3.15553
_cell_length_c 7.54242
_cell_angle_alpha 90.00024
_cell_angle_beta 89.99976
_cell_angle_gamma 120.00091
_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
Nb1 1.0 0.333334 0.666666 0.332848 Biso 1.000000 Nb
Nb2 1.0 0.666666 0.333334 0.667152 Biso 1.000000 Nb
C1 1.0 0.000000 0.000000 0.500000 Biso 1.000000 C
O1 1.0 0.666666 0.333334 0.189474 Biso 1.000000 O
O2 1.0 0.333334 0.666666 0.810527 Biso 1.000000 O

Nb₂C(OH)₂

```
#=====

# CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name      'XCrySDen XSF file'
_cell_length_a      3.23573
_cell_length_b      3.23574
_cell_length_c      7.84372
_cell_angle_alpha   89.99763
_cell_angle_beta    90.00233
_cell_angle_gamma   120.00032
_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
Nb1      1.0  0.666677  0.333323  0.641933  Biso 1.000000 Nb
Nb2      1.0  0.333323  0.666677  0.358079  Biso 1.000000 Nb
C1       1.0 -0.000000 -0.000000  0.500011  Biso 1.000000 C
O1       1.0  0.666666  0.333335  0.178003  Biso 1.000000 O
O2       1.0  0.333335  0.666664  0.821990  Biso 1.000000 O
H1       1.0  0.666660  0.333341  0.053451  Biso 1.000000 H
H2       1.0  0.333340  0.666659  0.946532  Biso 1.000000 H
```

Sc₂CF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.29129
_cell_length_b 3.29129
_cell_length_c 7.25692
_cell_angle_alpha 90.00047
_cell_angle_beta 89.99960
_cell_angle_gamma 120.00713
_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
Sc1 1.0 0.333336 0.666663 0.325428 Biso 1.000000 Sc
Sc2 1.0 0.666664 0.333337 0.674572 Biso 1.000000 Sc
C1 1.0 0.000000 0.000000 0.500000 Biso 1.000000 C
F1 1.0 0.666662 0.333336 0.168829 Biso 1.000000 F
F2 1.0 0.333338 0.666664 0.831171 Biso 1.000000 F

Sc₂C(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.29534
_cell_length_b 3.29534
_cell_length_c 7.91527
_cell_angle_alpha 90.00195
_cell_angle_beta 89.99803
_cell_angle_gamma 120.00808
_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
Sc1 1.0 0.666654 0.333346 0.659623 Biso 1.000000 Sc
Sc2 1.0 0.333346 0.666654 0.340377 Biso 1.000000 Sc
C1 1.0 0.000000 -0.000000 0.500000 Biso 1.000000 C
O1 1.0 0.666655 0.333345 0.182122 Biso 1.000000 O
O2 1.0 0.333344 0.666655 0.817880 Biso 1.000000 O
H1 1.0 0.666662 0.333338 0.059220 Biso 1.000000 H
H2 1.0 0.333338 0.666662 0.940777 Biso 1.000000 H

Ta₂CF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.20961
_cell_length_b 3.20961
_cell_length_c 7.51010
_cell_angle_alpha 90.00028
_cell_angle_beta 89.99975
_cell_angle_gamma 120.00146
_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
Ta1 1.0 0.333339 0.666661 0.355864 Biso 1.000000 Ta
Ta2 1.0 0.666662 0.333339 0.644136 Biso 1.000000 Ta
C1 1.0 -0.000000 -0.000000 0.499999 Biso 1.000000 C
F1 1.0 0.666654 0.333345 0.170655 Biso 1.000000 F
F2 1.0 0.333346 0.666655 0.829346 Biso 1.000000 F

Ta₂CO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name	'XCrySDen XSF file'						
_cell_length_a	3.13200						
_cell_length_b	3.13200						
_cell_length_c	7.59657						
_cell_angle_alpha	89.99973						
_cell_angle_beta	90.00032						
_cell_angle_gamma	119.99961						
_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							
Ta1	1.0	0.333330	0.666670	0.336327	Biso	1.000000	Ta
Ta2	1.0	0.666670	0.333330	0.663673	Biso	1.000000	Ta
C1	1.0	0.000000	0.000000	0.500000	Biso	1.000000	C
O1	1.0	0.666667	0.333332	0.194024	Biso	1.000000	O
O2	1.0	0.333333	0.666668	0.805976	Biso	1.000000	O

Ta₂C(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name	'XCrySDen XSF file'					
_cell_length_a	5.25008					
_cell_length_b	3.03591					
_cell_length_c	9.23742					
_cell_angle_alpha	90					
_cell_angle_beta	100.76468					
_cell_angle_gamma	90					
_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						
Ta1	1.0	0.714070	0.000000	0.145572	Biso	1.000000 Ta
Ta2	1.0	0.285938	0.000000	0.854434	Biso	1.000000 Ta
Ta3	1.0	0.214047	0.500000	0.145564	Biso	1.000000 Ta
Ta4	1.0	0.785947	0.500000	0.854432	Biso	1.000000 Ta
C1	1.0	0.500001	0.500000	-0.000001	Biso	1.000000 C
C2	1.0	-0.000001	0.000000	0.000000	Biso	1.000000 C
O1	1.0	0.096920	0.000000	0.295402	Biso	1.000000 O
O2	1.0	0.903072	0.000000	0.704583	Biso	1.000000 O
O3	1.0	0.596924	0.500000	0.295421	Biso	1.000000 O
O4	1.0	0.403082	0.500000	0.704593	Biso	1.000000 O
H1	1.0	0.132699	0.000000	0.404782	Biso	1.000000 H
H2	1.0	0.867295	0.000000	0.595201	Biso	1.000000 H
H3	1.0	0.632706	0.500000	0.404804	Biso	1.000000 H
H4	1.0	0.367301	0.500000	0.595213	Biso	1.000000 H

Ti₂CF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.05935
_cell_length_b 3.05935
_cell_length_c 7.54049
_cell_angle_alpha 90.00016
_cell_angle_beta 89.99984
_cell_angle_gamma 120.00045
_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
Ti1 1.0 0.333333 0.666668 0.348272 Biso 1.000000 Ti
Ti2 1.0 0.666668 0.333332 0.651729 Biso 1.000000 Ti
C1 1.0 0.000000 -0.000000 0.500000 Biso 1.000000 C
F1 1.0 0.666667 0.333333 0.183696 Biso 1.000000 F
F2 1.0 0.333333 0.666666 0.816304 Biso 1.000000 F

Ti₂CO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.03519
_cell_length_b 3.03519
_cell_length_c 7.60702
_cell_angle_alpha 90.00246
_cell_angle_beta 89.99759
_cell_angle_gamma 119.99790
_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
Ti1 1.0 0.333309 0.666690 0.328171 Biso 1.000000 Ti
Ti2 1.0 0.666691 0.333309 0.671829 Biso 1.000000 Ti
C1 1.0 -0.000000 0.000000 0.500000 Biso 1.000000 C
O1 1.0 0.666677 0.333321 0.207491 Biso 1.000000 O
O2 1.0 0.333323 0.666678 0.792509 Biso 1.000000 O

Ti₂C(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.09163
_cell_length_b 3.09163
_cell_length_c 7.65200
_cell_angle_alpha 90
_cell_angle_beta 90.00001
_cell_angle_gamma 120.00067
_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
Ti1 1.0 0.666668 0.333332 0.648176 Biso 1.000000 Ti
Ti2 1.0 0.333332 0.666668 0.351823 Biso 1.000000 Ti
C1 1.0 0.000000 0.000000 0.499998 Biso 1.000000 C
O1 1.0 0.666664 0.333335 0.183493 Biso 1.000000 O
O2 1.0 0.333336 0.666665 0.816508 Biso 1.000000 O
H1 1.0 0.666667 0.333333 0.056227 Biso 1.000000 H
H2 1.0 0.333333 0.666667 0.943775 Biso 1.000000 H

Ti₂NF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.07137
_cell_length_b 3.07137
_cell_length_c 7.34636
_cell_angle_alpha 90.00109
_cell_angle_beta 89.99891
_cell_angle_gamma 120.00262
_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
Ti1 1.0 0.333329 0.666671 0.354118 Biso 1.000000 Ti
Ti2 1.0 0.666671 0.333329 0.645882 Biso 1.000000 Ti
N1 1.0 0.000000 0.000000 0.500000 Biso 1.000000 N
F1 1.0 0.666666 0.333334 0.185794 Biso 1.000000 F
F2 1.0 0.333334 0.666666 0.814206 Biso 1.000000 F

Ti₂NO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.00343
_cell_length_b 3.00343
_cell_length_c 7.55852
_cell_angle_alpha 90.00095
_cell_angle_beta 89.99913
_cell_angle_gamma 119.99907
_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
Ti1 1.0 0.333322 0.666678 0.332319 Biso 1.000000 Ti
Ti2 1.0 0.666678 0.333322 0.667678 Biso 1.000000 Ti
N1 1.0 -0.000000 0.000000 0.500001 Biso 1.000000 N
O1 1.0 0.666672 0.333326 0.205945 Biso 1.000000 O
O2 1.0 0.333328 0.666674 0.794058 Biso 1.000000 O

Ti₂N(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name	'XCrySDen XSF file'				
_cell_length_a	3.08439				
_cell_length_b	3.08439				
_cell_length_c	7.54999				
_cell_angle_alpha	90.00009				
_cell_angle_beta	89.99990				
_cell_angle_gamma	120.00043				
_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					
Ti1	1.0	0.666667	0.333333	0.643528	Biso 1.000000 Ti
Ti2	1.0	0.333333	0.666667	0.356472	Biso 1.000000 Ti
N1	1.0	-0.000000	0.000000	0.500001	Biso 1.000000 N
O1	1.0	0.666664	0.333336	0.187151	Biso 1.000000 O
O2	1.0	0.333335	0.666664	0.812848	Biso 1.000000 O
H1	1.0	0.666666	0.333334	0.058113	Biso 1.000000 H
H2	1.0	0.333333	0.666666	0.941887	Biso 1.000000 H

V₂CF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 2.98839
_cell_length_b 2.98839
_cell_length_c 7.44649
_cell_angle_alpha 90.00146
_cell_angle_beta 89.99865
_cell_angle_gamma 120.00095
_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
V1 1.0 0.333331 0.666668 0.362813 Biso 1.000000 V
V2 1.0 0.666669 0.333332 0.637187 Biso 1.000000 V
C1 1.0 0.000000 -0.000000 0.500000 Biso 1.000000 C
F1 1.0 0.666667 0.333331 0.191851 Biso 1.000000 F
F2 1.0 0.333333 0.666670 0.808149 Biso 1.000000 F

V₂CO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 2.89639
_cell_length_b 2.89639
_cell_length_c 7.54158
_cell_angle_alpha 89.99985
_cell_angle_beta 90.00008
_cell_angle_gamma 119.99973
_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
V1 1.0 0.333332 0.666668 0.342167 Biso 1.000000 V
V2 1.0 0.666668 0.333331 0.657832 Biso 1.000000 V
C1 1.0 0.000000 -0.000000 0.500000 Biso 1.000000 C
O1 1.0 0.666668 0.333334 0.207239 Biso 1.000000 O
O2 1.0 0.333332 0.666666 0.792761 Biso 1.000000 O

V₂C(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.01040
_cell_length_b 3.01040
_cell_length_c 7.69889
_cell_angle_alpha 89.99993
_cell_angle_beta 89.99997
_cell_angle_gamma 119.99989
_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
V1 1.0 0.666665 0.333334 0.633340 Biso 1.000000 V
V2 1.0 0.333335 0.666666 0.366666 Biso 1.000000 V
C1 1.0 -0.000000 -0.000000 0.500001 Biso 1.000000 C
O1 1.0 0.666668 0.333334 0.200058 Biso 1.000000 O
O2 1.0 0.333332 0.666666 0.799940 Biso 1.000000 O
H1 1.0 0.666668 0.333333 0.073333 Biso 1.000000 H
H2 1.0 0.333332 0.666668 0.926662 Biso 1.000000 H

Zr₂CF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.31813
_cell_length_b 3.31813
_cell_length_c 7.34665
_cell_angle_alpha 90.05552
_cell_angle_beta 89.94435
_cell_angle_gamma 120.19835
_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
Zr1 1.0 0.333047 0.666954 0.341891 Biso 1.000000 Zr
Zr2 1.0 0.666953 0.333046 0.658109 Biso 1.000000 Zr
N1 1.0 -0.000000 -0.000000 0.500000 Biso 1.000000 N
F1 1.0 0.666629 0.333374 0.164286 Biso 1.000000 F
F2 1.0 0.333371 0.666626 0.835714 Biso 1.000000 F

Zr₂CO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.28506
_cell_length_b 3.28506
_cell_length_c 7.05971
_cell_angle_alpha 89.99775
_cell_angle_beta 90.00225
_cell_angle_gamma 120.00877
_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
Zr1 1.0 0.333403 0.666598 0.307932 Biso 1.000000 Zr
Zr2 1.0 0.666598 0.333402 0.692068 Biso 1.000000 Zr
N1 1.0 0.000000 0.000000 0.500000 Biso 1.000000 N
O1 1.0 0.666628 0.333372 0.170433 Biso 1.000000 O
O2 1.0 0.333372 0.666628 0.829567 Biso 1.000000 O

Zr₂C(OH)₂

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.29554
_cell_length_b 3.29613
_cell_length_c 9.88035
_cell_angle_alpha 90.38525
_cell_angle_beta 87.90900
_cell_angle_gamma 120.01154
_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
Zr1 1.0 0.336266 0.524512 0.808233 Biso 1.000000 Zr
Zr2 1.0 0.635375 0.179252 0.066416 Biso 1.000000 Zr
C1 1.0 0.986551 0.852152 0.932258 Biso 1.000000 C
O1 1.0 0.687615 0.197400 0.672192 Biso 1.000000 O
O2 1.0 0.950706 0.839626 0.203933 Biso 1.000000 O
H1 1.0 0.700037 0.201414 0.572726 Biso 1.000000 H
H2 1.0 0.937520 0.835634 0.303229 Biso 1.000000 H

Zr₂NF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.31813
_cell_length_b 3.31813
_cell_length_c 7.34665
_cell_angle_alpha 90.05552
_cell_angle_beta 89.94435
_cell_angle_gamma 120.19835
_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
Zr1 1.0 0.333047 0.666954 0.341891 Biso 1.000000 Zr
Zr2 1.0 0.666953 0.333046 0.658109 Biso 1.000000 Zr
N1 1.0 -0.000000 -0.000000 0.500000 Biso 1.000000 N
F1 1.0 0.666629 0.333374 0.164286 Biso 1.000000 F
F2 1.0 0.333371 0.666626 0.835714 Biso 1.000000 F

Zr₂NO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.31813
_cell_length_b 3.31813
_cell_length_c 7.34665
_cell_angle_alpha 90.05552
_cell_angle_beta 89.94435
_cell_angle_gamma 120.19835
_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
Zr1 1.0 0.333047 0.666954 0.341891 Biso 1.000000 Zr
Zr2 1.0 0.666953 0.333046 0.658109 Biso 1.000000 Zr
N1 1.0 -0.000000 -0.000000 0.500000 Biso 1.000000 N
F1 1.0 0.666629 0.333374 0.164286 Biso 1.000000 F
F2 1.0 0.333371 0.666626 0.835714 Biso 1.000000 F

Zr₂N(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.29001
_cell_length_b 3.29001
_cell_length_c 8.61206
_cell_angle_alpha 89.98775
_cell_angle_beta 90.01230
_cell_angle_gamma 120.00282
_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
Zr1 1.0 0.666731 0.333270 0.639938 Biso 1.000000 Zr
Zr2 1.0 0.333269 0.666730 0.360062 Biso 1.000000 Zr
N1 1.0 0.000000 -0.000000 0.500000 Biso 1.000000 N
O1 1.0 0.666543 0.333455 0.207763 Biso 1.000000 O
O2 1.0 0.333457 0.666545 0.792238 Biso 1.000000 O
H1 1.0 0.666577 0.333422 0.093309 Biso 1.000000 H
H2 1.0 0.333424 0.666578 0.906690 Biso 1.000000 H

Mo₂CF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.27837
_cell_length_b 3.27837
_cell_length_c 7.14471
_cell_angle_alpha 89.99997
_cell_angle_beta 90.00002
_cell_angle_gamma 120.00123
_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
Mo1 1.0 0.333333 0.666667 0.367906 Biso 1.000000 Mo
Mo2 1.0 0.666667 0.333333 0.632094 Biso 1.000000 Mo
C1 1.0 -0.000000 -0.000000 0.500000 Biso 1.000000 C
F1 1.0 0.666667 0.333333 0.184421 Biso 1.000000 F
F2 1.0 0.333333 0.666667 0.815579 Biso 1.000000 F

Mo₂CCl₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.36565
_cell_length_b 3.36565
_cell_length_c 8.85054
_cell_angle_alpha 90.00171
_cell_angle_beta 89.99828
_cell_angle_gamma 120.00412
_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
Mo1 1.0 0.333324 0.666676 0.395078 Biso 1.000000 Mo
Mo2 1.0 0.666676 0.333324 0.604923 Biso 1.000000 Mo
Cl1 1.0 -0.000000 -0.000000 0.499997 Biso 1.000000 Cl
Cl2 1.0 0.666657 0.333343 0.195904 Biso 1.000000 Cl
Cl3 1.0 0.333343 0.666657 0.804098 Biso 1.000000 Cl

Mo₂CBr₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.41871
_cell_length_b 3.41871
_cell_length_c 9.19621
_cell_angle_alpha 90.00133
_cell_angle_beta 89.99867
_cell_angle_gamma 120.00288
_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
Mo1 1.0 0.333325 0.666675 0.401073 Biso 1.000000 Mo
Mo2 1.0 0.666675 0.333325 0.598932 Biso 1.000000 Mo
C1 1.0 0.000000 -0.000000 0.499988 Biso 1.000000 C
Br1 1.0 0.666659 0.333341 0.191356 Biso 1.000000 Br
Br2 1.0 0.333341 0.666659 0.808651 Biso 1.000000 Br

Mo₂C(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.29681
_cell_length_b 3.29681
_cell_length_c 7.24679
_cell_angle_alpha 90.01091
_cell_angle_beta 89.98909
_cell_angle_gamma 120.02212
_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
Mo1 1.0 0.666696 0.333304 0.630234 Biso 1.000000 Mo
Mo2 1.0 0.333304 0.666696 0.369764 Biso 1.000000 Mo
C1 1.0 -0.000000 0.000000 0.500000 Biso 1.000000 C
O1 1.0 0.666622 0.333378 0.187226 Biso 1.000000 O
O2 1.0 0.333377 0.666622 0.812776 Biso 1.000000 O
H1 1.0 0.666652 0.333348 0.052173 Biso 1.000000 H
H2 1.0 0.333348 0.666652 0.947825 Biso 1.000000 H

Mo₂CO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 4.99387
_cell_length_b 2.88681
_cell_length_c 11.08658
_cell_angle_alpha 90
_cell_angle_beta 130.78244
_cell_angle_gamma 90
_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
Mo1 1.0 0.428694 0.500000 0.336011 Biso 1.000000 Mo
Mo2 1.0 0.571306 0.500000 0.663989 Biso 1.000000 Mo
Mo3 1.0 0.928694 0.000000 0.336011 Biso 1.000000 Mo
Mo4 1.0 0.071306 0.000000 0.663989 Biso 1.000000 Mo
C1 1.0 0.500000 0.000000 0.500000 Biso 1.000000 C
C2 1.0 0.000000 0.500000 0.500000 Biso 1.000000 C
O1 1.0 0.050989 0.000000 0.190293 Biso 1.000000 O
O2 1.0 0.949011 0.000000 0.809707 Biso 1.000000 O
O3 1.0 0.550989 0.500000 0.190293 Biso 1.000000 O
O4 1.0 0.449011 0.500000 0.809707 Biso 1.000000 O

Mo₂CS₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 5.33770
_cell_length_b 3.07818
_cell_length_c 12.50083
_cell_angle_alpha 90
_cell_angle_beta 128.43141
_cell_angle_gamma 90
_symmetry_space_group_name_H-M 'P 1'
_symmetry_Int_Tables_number 1

loop_
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'x, y, z'

loop_
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_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
Mo1 1.0 0.474397 0.500000 0.367274 Biso 1.000000 Mo
Mo2 1.0 0.525603 0.500000 0.632726 Biso 1.000000 Mo
Mo3 1.0 -0.025605 0.000000 0.367274 Biso 1.000000 Mo
Mo4 1.0 0.025605 0.000000 0.632726 Biso 1.000000 Mo
C1 1.0 0.500001 0.000000 0.500000 Biso 1.000000 C
C2 1.0 -0.000001 0.500000 0.500000 Biso 1.000000 C
S1 1.0 0.067287 0.000000 0.202126 Biso 1.000000 S
S2 1.0 -0.067288 0.000000 0.797874 Biso 1.000000 S
S3 1.0 0.567288 0.500000 0.202127 Biso 1.000000 S
S4 1.0 0.432712 0.500000 0.797874 Biso 1.000000 S

Cr₂CF₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

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_cell_length_a 3.02478
_cell_length_b 3.02478
_cell_length_c 7.12929
_cell_angle_alpha 89.99720
_cell_angle_beta 90.00281
_cell_angle_gamma 119.99272
_symmetry_space_group_name_H-M 'P 1'
_symmetry_Int_Tables_number 1

loop_
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'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
Cr1 1.0 0.333347 0.666653 0.372917 Biso 1.000000 Cr
Cr2 1.0 0.666653 0.333347 0.627085 Biso 1.000000 Cr
C1 1.0 -0.000000 0.000000 0.499998 Biso 1.000000 C
F1 1.0 0.666672 0.333328 0.199428 Biso 1.000000 F
F2 1.0 0.333328 0.666672 0.800571 Biso 1.000000 F

Cr₂CCl₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.16170
_cell_length_b 3.16170
_cell_length_c 8.98370
_cell_angle_alpha 90.00050
_cell_angle_beta 89.99950
_cell_angle_gamma 120.00039
_symmetry_space_group_name_H-M 'P 1'
_symmetry_Int_Tables_number 1

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_symmetry_equiv_pos_as_xyz
'x, y, z'

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_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
Cr1 1.0 0.333331 0.666669 0.402779 Biso 1.000000 Cr
Cr2 1.0 0.666669 0.333332 0.597250 Biso 1.000000 Cr
C1 1.0 0.000000 -0.000000 0.499958 Biso 1.000000 C
Cl2 1.0 0.666666 0.333335 0.218958 Biso 1.000000 Cl
Cl3 1.0 0.333334 0.666666 0.781055 Biso 1.000000 Cl

Cr₂CBr₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.25680
_cell_length_b 3.25680
_cell_length_c 8.96334
_cell_angle_alpha 90.00082
_cell_angle_beta 89.99919
_cell_angle_gamma 120.00161
_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
Cr1 1.0 0.333326 0.666674 0.408403 Biso 1.000000 Cr
Cr2 1.0 0.666674 0.333326 0.591597 Biso 1.000000 Cr
C1 1.0 0.000000 0.000000 0.500001 Biso 1.000000 C
Br1 1.0 0.666665 0.333335 0.205806 Biso 1.000000 Br
Br2 1.0 0.333335 0.666665 0.794192 Biso 1.000000 Br

Cr₂C(OH)₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 3.05246
_cell_length_b 3.05246
_cell_length_c 7.12331
_cell_angle_alpha 90.00044
_cell_angle_beta 89.99953
_cell_angle_gamma 120.00087
_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
Cr1 1.0 0.666668 0.333332 0.627152 Biso 1.000000 Cr
Cr2 1.0 0.333332 0.666668 0.372843 Biso 1.000000 Cr
C1 1.0 -0.000000 -0.000000 0.499997 Biso 1.000000 C
O1 1.0 0.666666 0.333334 0.198338 Biso 1.000000 O
O2 1.0 0.333334 0.666665 0.801665 Biso 1.000000 O
H1 1.0 0.666667 0.333333 0.061228 Biso 1.000000 H
H2 1.0 0.333333 0.666666 0.938777 Biso 1.000000 H

Cr₂CO₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

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_cell_length_a 4.66366
_cell_length_b 2.69355
_cell_length_c 10.40718
_cell_angle_alpha 90
_cell_angle_beta 130.52524
_cell_angle_gamma 90
_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
Cr1 1.0 0.430858 0.500000 0.337392 Biso 1.000000 Cr
Cr2 1.0 0.569141 0.500000 0.662607 Biso 1.000000 Cr
Cr3 1.0 0.930858 0.000000 0.337392 Biso 1.000000 Cr
Cr4 1.0 0.069142 0.000000 0.662608 Biso 1.000000 Cr
C1 1.0 0.500000 0.000000 0.500000 Biso 1.000000 C
C2 1.0 -0.000000 0.500000 0.500000 Biso 1.000000 C
O1 1.0 0.057361 0.000000 0.194716 Biso 1.000000 O
O2 1.0 0.942641 0.000000 0.805284 Biso 1.000000 O
O3 1.0 0.557360 0.500000 0.194716 Biso 1.000000 O
O4 1.0 0.442640 0.500000 0.805284 Biso 1.000000 O

Cr₂CS₂

#=====

CRYSTAL DATA

#-----

data_VESTA_phase_1

_pd_phase_name 'XCrySDen XSF file'
_cell_length_a 5.07788
_cell_length_b 2.93352
_cell_length_c 12.09970
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_cell_angle_gamma 90
_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
Cr1 1.0 0.489461 0.500000 0.378723 Biso 1.000000 Cr
Cr2 1.0 0.510539 0.500000 0.621272 Biso 1.000000 Cr
Cr3 1.0 0.989459 0.000000 0.378719 Biso 1.000000 Cr
Cr4 1.0 0.010538 0.000000 0.621283 Biso 1.000000 Cr
C1 1.0 0.499993 0.000000 0.500002 Biso 1.000000 C
C2 1.0 0.000008 0.500000 0.499999 Biso 1.000000 C
S1 1.0 0.089343 0.000000 0.218860 Biso 1.000000 S
S2 1.0 0.910656 0.000000 0.781140 Biso 1.000000 S
S3 1.0 0.589355 0.500000 0.218860 Biso 1.000000 S
S4 1.0 0.410649 0.500000 0.781141 Biso 1.000000 S

A justification why we have used constant relaxation time approximation in our thermoelectric calculations on MXenes

The relaxation time (τ) can be determined by electron-electron and electron-phonon scattering, which depend on the electron band structure and phonon dispersions. However, obtaining relaxation time from theory is very difficult and tedious task because it requires a deep knowledge about all possible scattering mechanisms by electrons, phonons, impurities and vacancies and so on. Owing to the above difficulties, the accepted approach in the literature is based on considering relaxation time as a constant and estimating it as a fitting parameter to the electrical conductivity measurements (e.g., please see the paper by J. Yang et al., *Phys. Rev. B* 2011, **84**, 235205). Therefore, the resulting relaxation time is considered as an effective parameter incorporating all scattering mechanisms. Unfortunately, at present there are no experimental electrical conductivity measurements to estimate the relaxation time for the MXenes. However, fortunately we have some experimental data for the electrical conductivity of the precursors of MXenes, i.e., M_2AX phases. We have extensively searched the litterateur and found the electrical conductivity data (σ) for 16 different M_2AX systems. In the following Table, we have shown all the experimental data obtained by different experimental groups and maybe different experimental conditions. Still the number of available experimental data is very limited. These experimental data sometimes have large differences.

We have constructed the M_2AX models. By using Boltzmann theory and first-principles calculations, we calculated the σ/τ for M_2AX systems (please see following Figure) and through fitting to the experimental data of σ , we have estimated τ (please see the following Table). It is seen that the calculated lattice parameters of M_2AX are in good agreement with the experimental results. It is seen that the estimated relaxation time falls in the range between $(0.4-2.7) \times 10^{-14}$ s. Despite limitations in the number of experimental conductivity measurements and their scattered data for different M_2AX systems, which include various transition metals (M), and different interlayer elements (A) and X atoms (carbon or nitrogen), still it can be concluded that the relaxation time $\sim 1.251 \times 10^{-14}$ s can be a reliable value for the relaxation time for all the considered M_2AX systems with similar hexagonal structures. Structurally MXenes are similar to MAX phases, but simpler because “A” element is absent.

Therefore, the variation of relaxation time for MXene systems might fall into a smaller range than for M₂AX systems. This was the reason why we expected “the relaxation time of different MXenes is in the same order”.

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M ₂ AX Phase	a (Å)	c (Å)	Experimental σ (1/ $\mu\Omega\cdot\text{m}$)	Calculated σ/τ (1/ $\Omega\cdot\text{m}\cdot\text{s}$)	Estimated τ (s)
Ti ₂ AlC	3.069, 3.051 ¹	13.737, 13.637 ¹	2.7 ^{1,2} , 2.8 ¹	2.797×10 ²⁰	1.036×10 ⁻¹⁴ , 0.999×10 ⁻¹⁴
Ti ₂ AlN	2.997, 2.989 ¹	13.644, 13.614 ¹	3.2 ³ , 4.00 ¹	2.700×10 ²⁰	0.844×10 ⁻¹⁴ , 0.675×10 ⁻¹⁴
Ti ₂ SC	3.205, 3.216 ⁴	11.257, 11.22 ⁴	1.923 ⁵	1.450×10 ²⁰	0.754×10 ⁻¹⁴
Ti ₂ GeC	3.094, 3.07 ⁴	12.991, 12.93 ⁴	4.4 ³	3.995×10 ²⁰	0.908×10 ⁻¹⁴
Ti ₂ InC	3.148, 3.134 ⁴	14.208, 14.077 ⁴	5.000 ⁶	2.367×10 ²⁰	0.473×10 ⁻¹⁴
Ti ₂ SnC	3.178, 3.163 ⁴	13.777, 13.679 ⁴	4.545 ⁷	3.944×10 ²⁰	0.868×10 ⁻¹⁴
V ₂ AlC	2.906, 3.1 ⁴	13.104, 13.83 ⁴	4.000 ⁸	3.095×10 ²⁰	0.774×10 ⁻¹⁴
Cr ₂ AlC	2.847, 2.863 ²	12.671, 12.814 ²	1.389 ⁸ , 1.4 ²	2.998×10 ²⁰	2.129×10 ⁻¹⁴ , 2.158×10 ⁻¹⁴
Zr ₂ SnC	3.390, 3.358 ⁴	14.684, 14.57 ⁴	3.571 ⁷ , 7.00 ⁹	4.475×10 ²⁰	1.253×10 ⁻¹⁴ , 0.639×10 ⁻¹⁴
Zr ₂ PbC	3.418, 3.38 ⁴	14.926, 14.66 ⁴	2.778 ⁷	4.455×10 ²⁰	1.604×10 ⁻¹⁴
Nb ₂ AlC	3.116, 3.1 ⁴	13.932, 13.8 ⁴	3.448 ¹⁰	4.174×10 ²⁰	1.210×10 ⁻¹⁴
Nb ₂ SnC	3.268, 3.214 ⁴	13.888, 13.802 ⁴	2.222 ⁷ , 4.00 ⁹	6.070×10 ²⁰	2.732×10 ⁻¹⁴ , 1.517×10 ⁻¹⁴
Hf ₂ InC	3.324, 3.309	14.890, 14.723	5.263 ⁶	3.270×10 ²⁰	0.621×10 ⁻¹⁴
Hf ₂ SnC	3.345, 3.320 ⁴	14.449, 14.388 ⁴	2.222 ⁷ , 2.4 ⁹	5.379×10 ²⁰	2.421×10 ⁻¹⁴ , 2.241×10 ⁻¹⁴
Hf ₂ PbC	3.379, 3.55 ⁷	14.680, 14.46 ⁷	13.333 ⁷	5.391×10 ²⁰	0.404×10 ⁻¹⁴
Ta ₂ AlC	3.093, 3.079 ¹¹	13.957, 13.860 ¹¹	3.91 ¹²	4.803×10 ²⁰	1.228×10 ⁻¹⁴

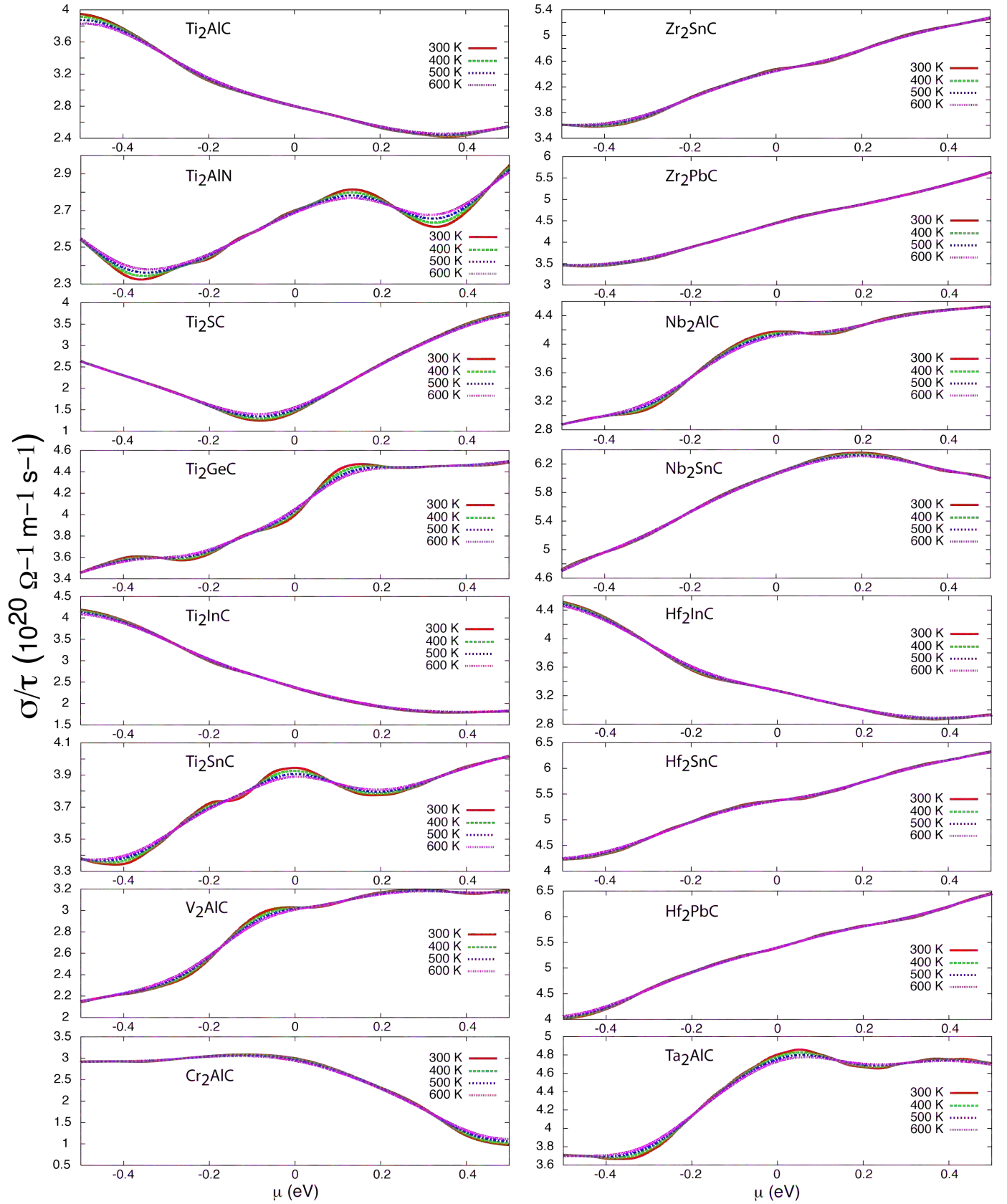


Figure 1: The calculated conductivity for various M_2AX systems as a function of chemical potential at different temperature.