Supplemental information

The Combined Influence of Dopant Species and Surface Termination on the Electronic Properties of Diamond Surfaces

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Figure S1

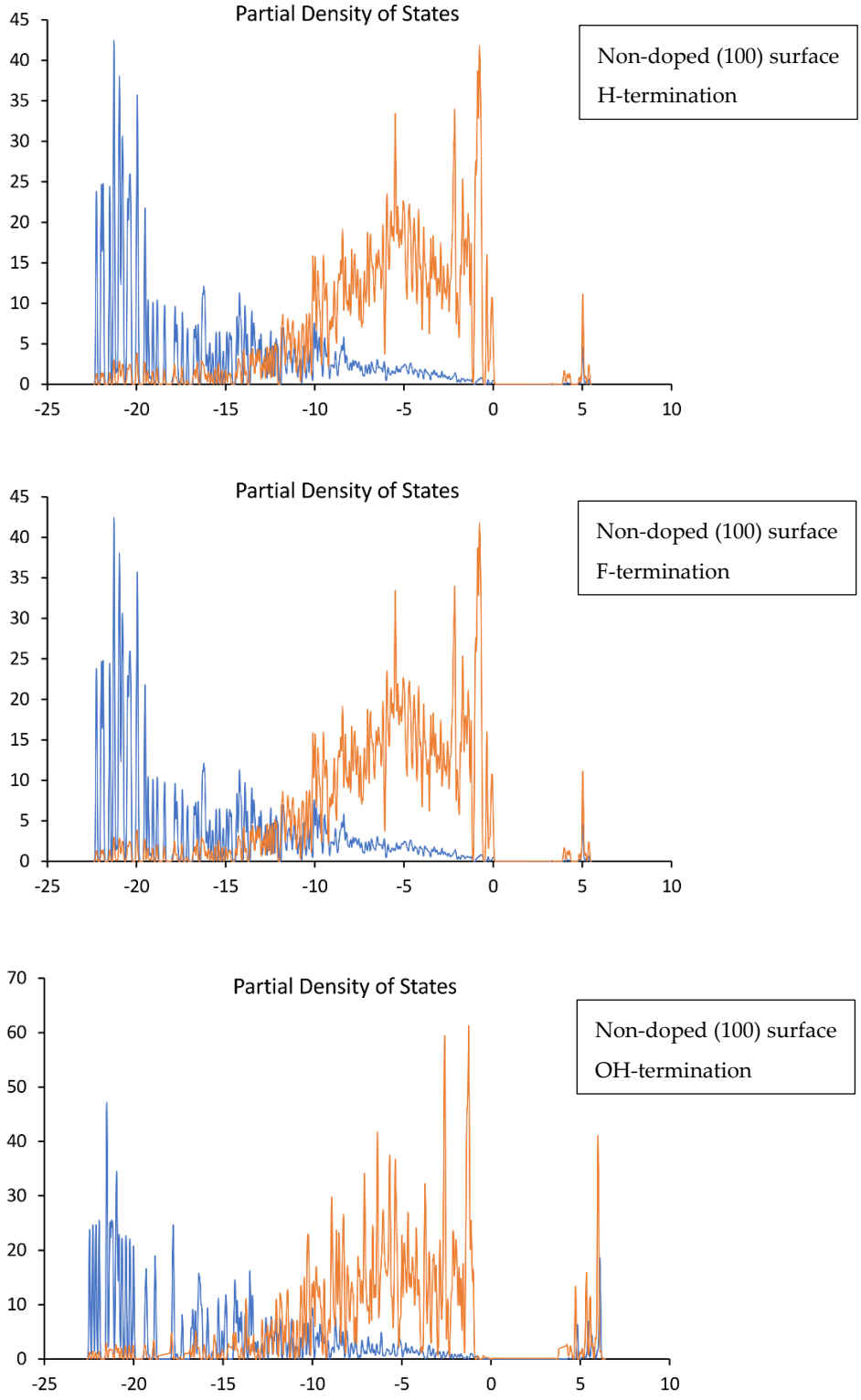
Partial Density of States
Non-doped (100) surface
H-termination
Partial Density of States
Non-doped (100) surface
F-termination
Partial Density of States
Non-doped (100) surface
OH-termination

Figure S1 (cont.)

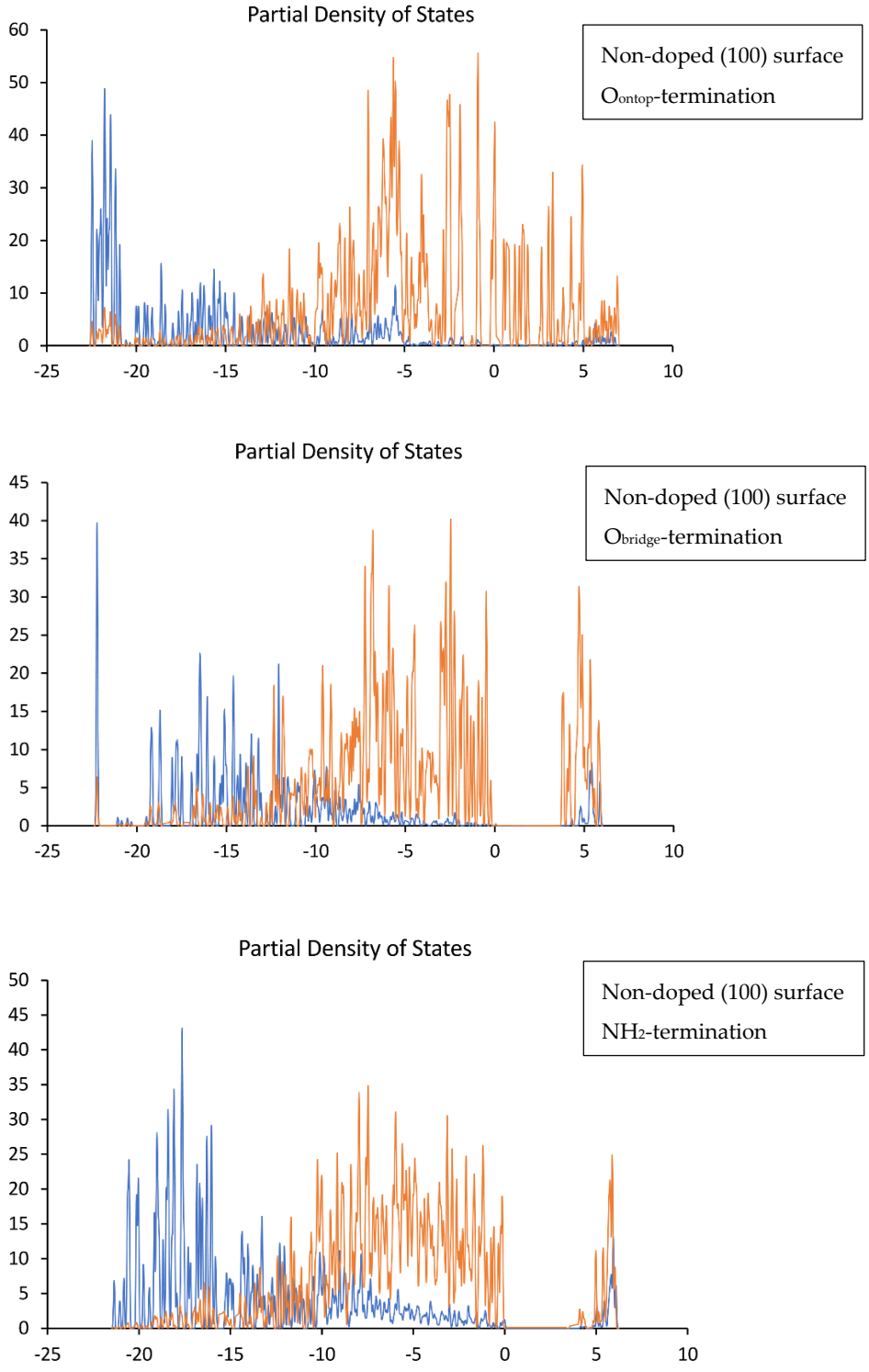

Figure S1. Calculated DOS spectra for non-doped terminated (100) surfaces. The spectra cover the upper surface parts (i.e., terminating layer and C atoms in the upper two atomic layers). The unit of the x-axis is eV, and the unit of the y-axis is electron density. The Fermi level is positioned at 0 eV. Blue: s-states; Orange: p-states.

Figure S2

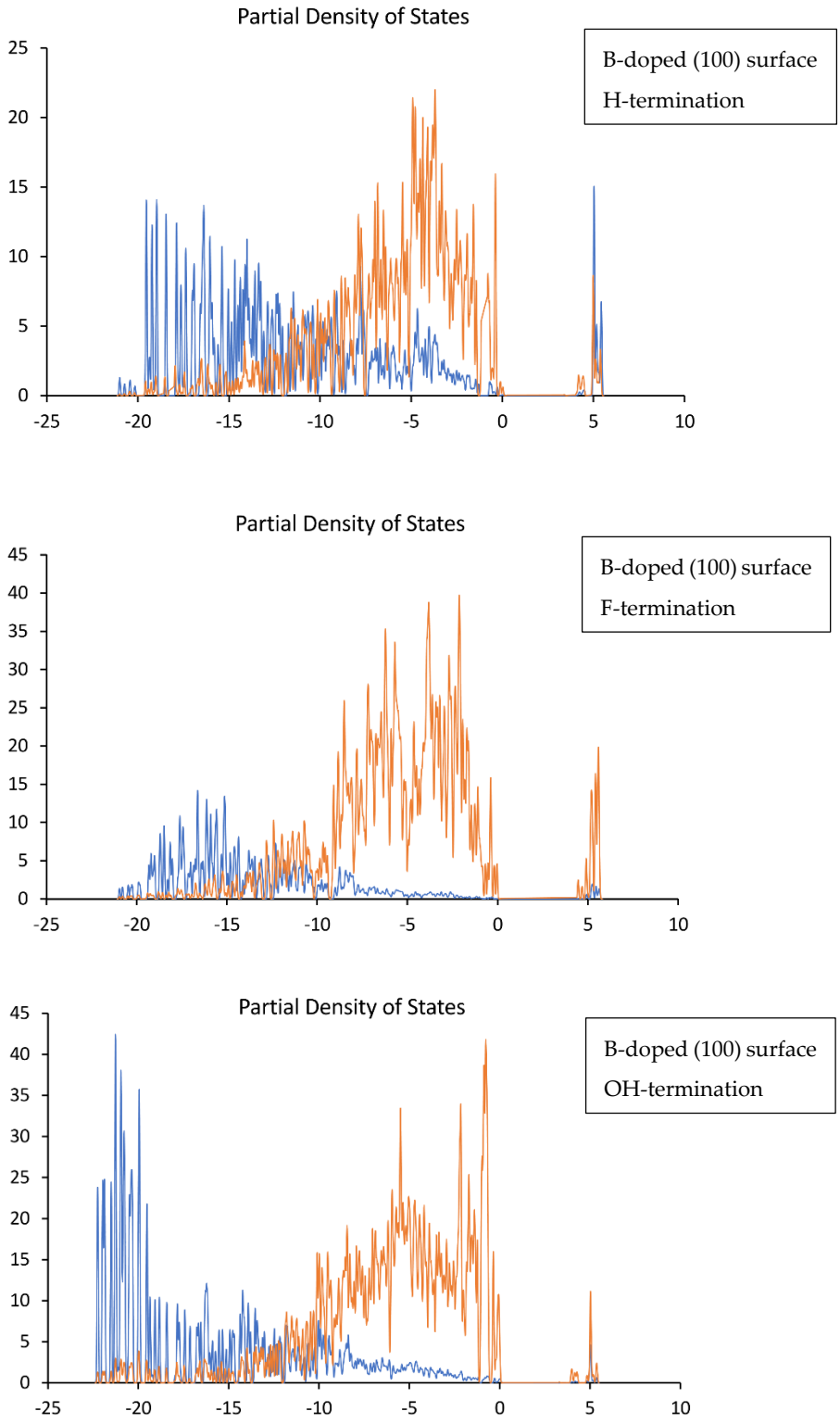
Partial Density of States
B-doped (100) surface
H-termination
Partial Density of States
B-doped (100) surface
F-termination
Partial Density of States
B-doped (100) surface
OH-termination

Figure S2 (cont.)

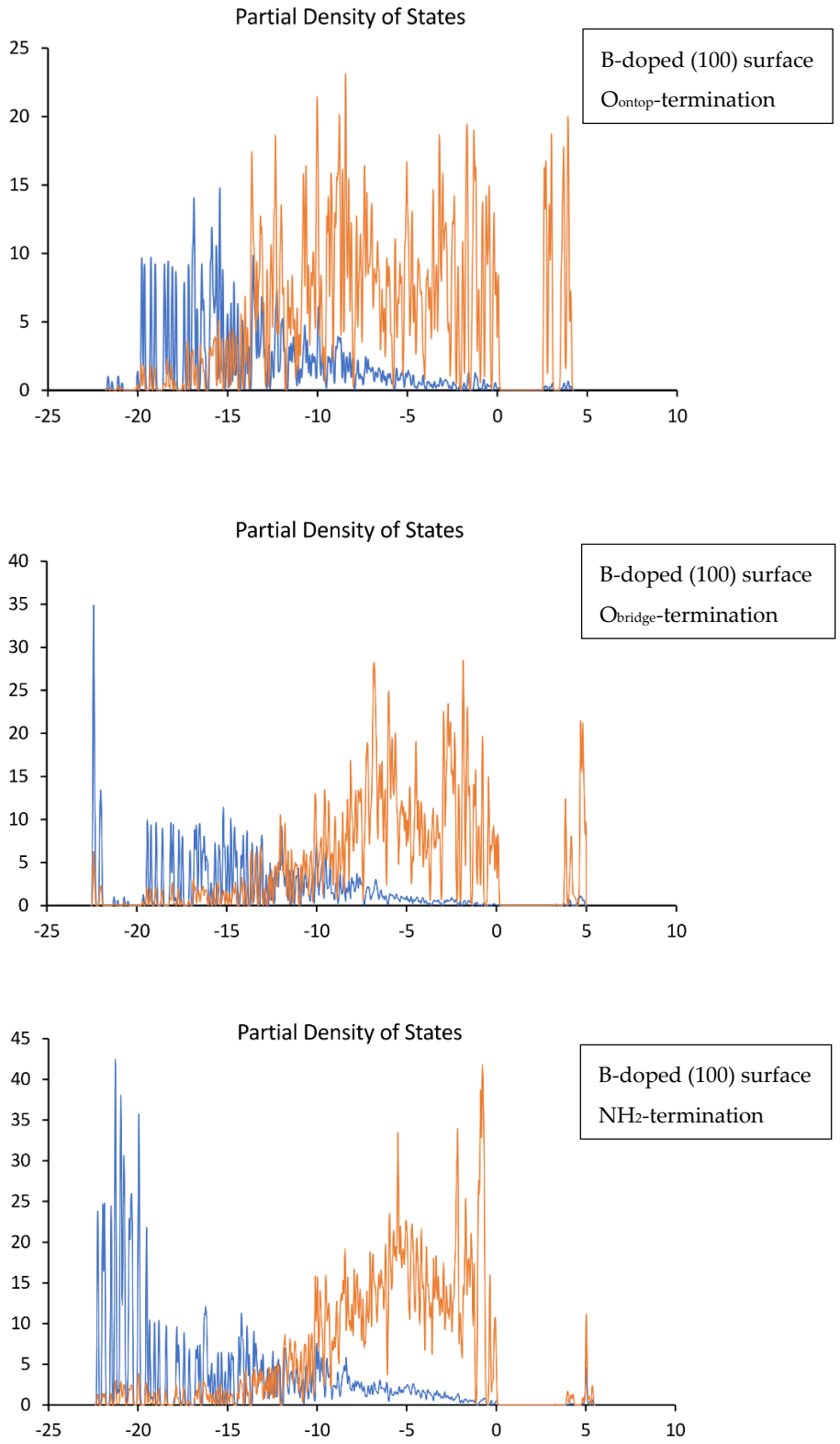

Figure S2. Calculated DOS spectra for B-doped terminated (100) surfaces. The spectra cover the upper surface parts (i.e., terminating layer and C atoms in the upper two atomic layers). The unit of the x-axis is eV, and the unit of the y-axis is electron density. The Fermi level is positioned at 0 eV. Blue: s-states; Orange: p-states.

Figure S3

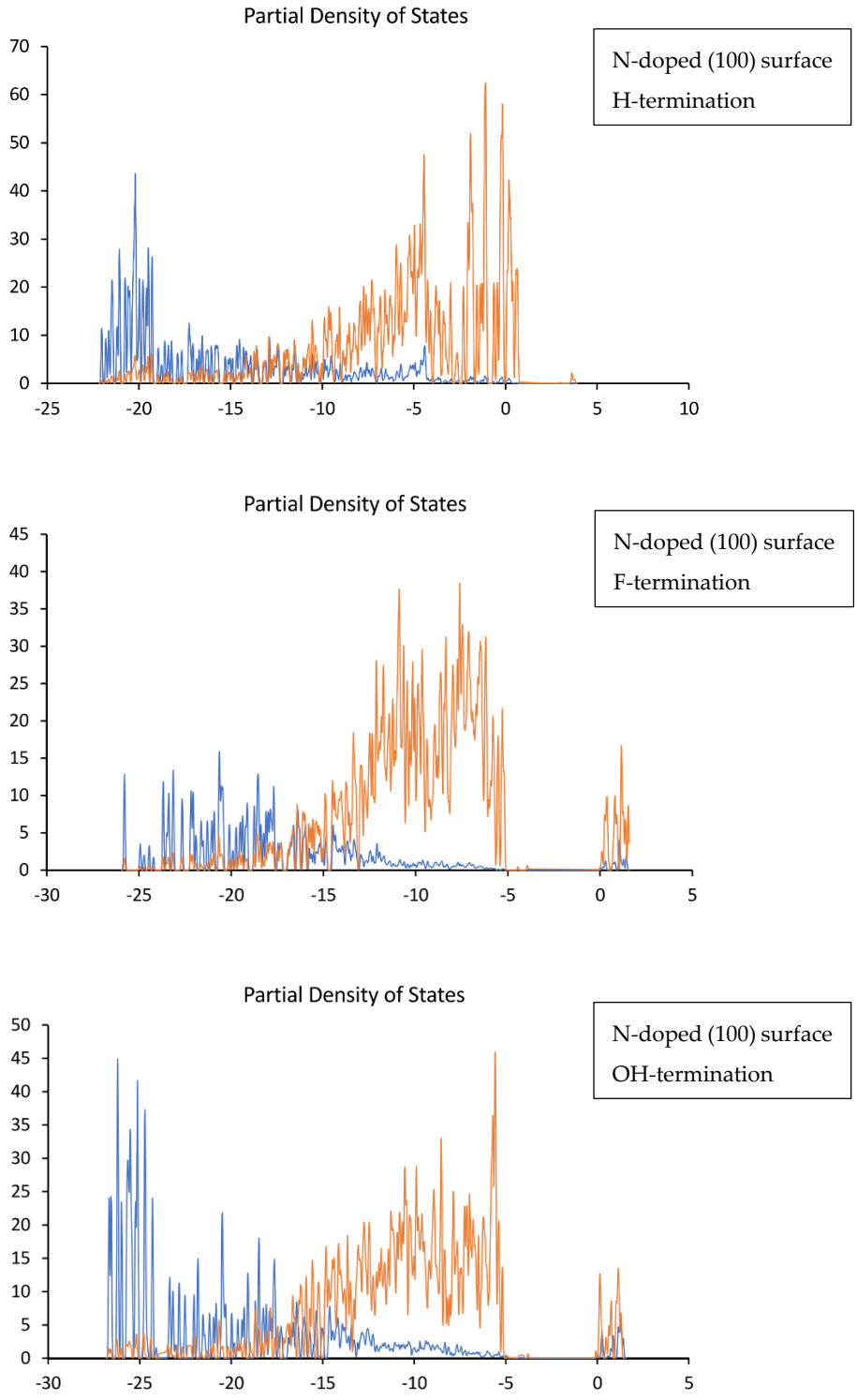
Partial Density of States
N-doped (100) surface
H-termination
Partial Density of States
N-doped (100) surface
F-termination
Partial Density of States
N-doped (100) surface
OH-termination

Figure S3 (cont.)

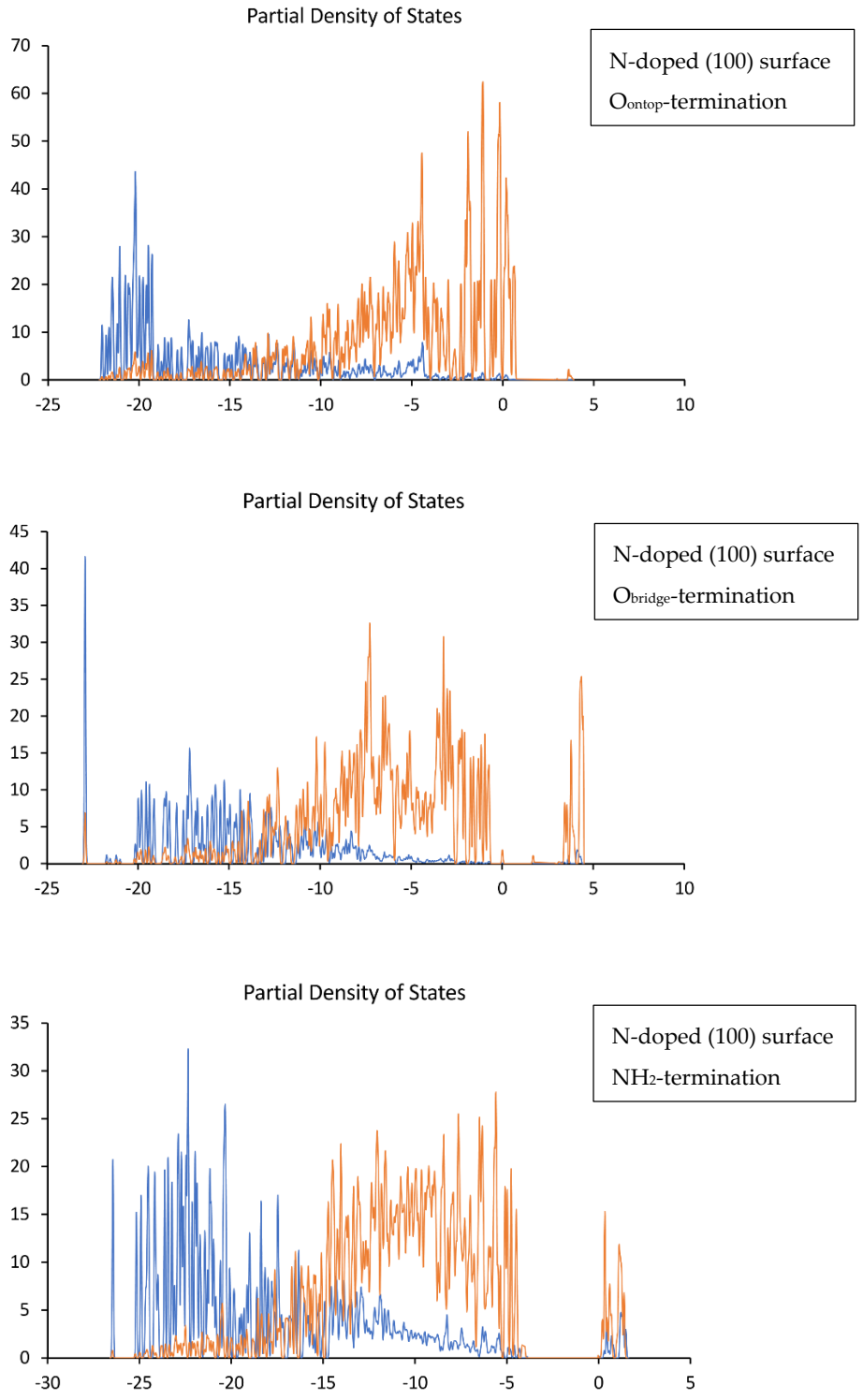

Figure S3. Calculated DOS spectra for N-doped terminated (100) surfaces. The spectra cover the upper surface parts (i.e., terminating layer and C atoms in the upper two atomic layers). The unit of the x-axis is eV, and the unit of the y-axis is electron density. The Fermi level is positioned at 0 eV. Blue: s-states; Orange: p-states.

Figure S4

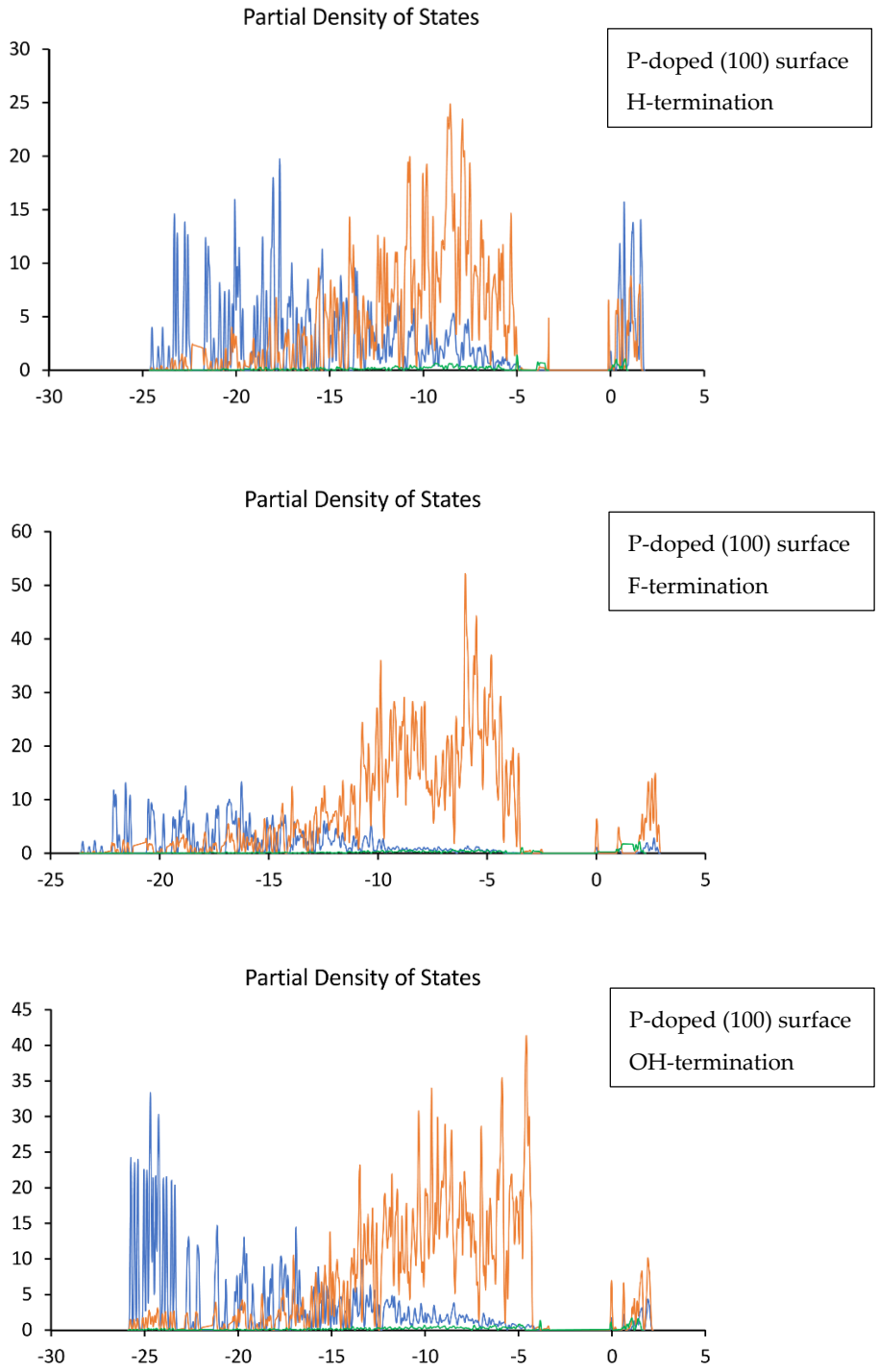
Partial Density of States
P-doped (100) surface
H-termination
Partial Density of States
P-doped (100) surface
F-termination
Partial Density of States
P-doped (100) surface
OH-termination

Figure S4 (cont.)

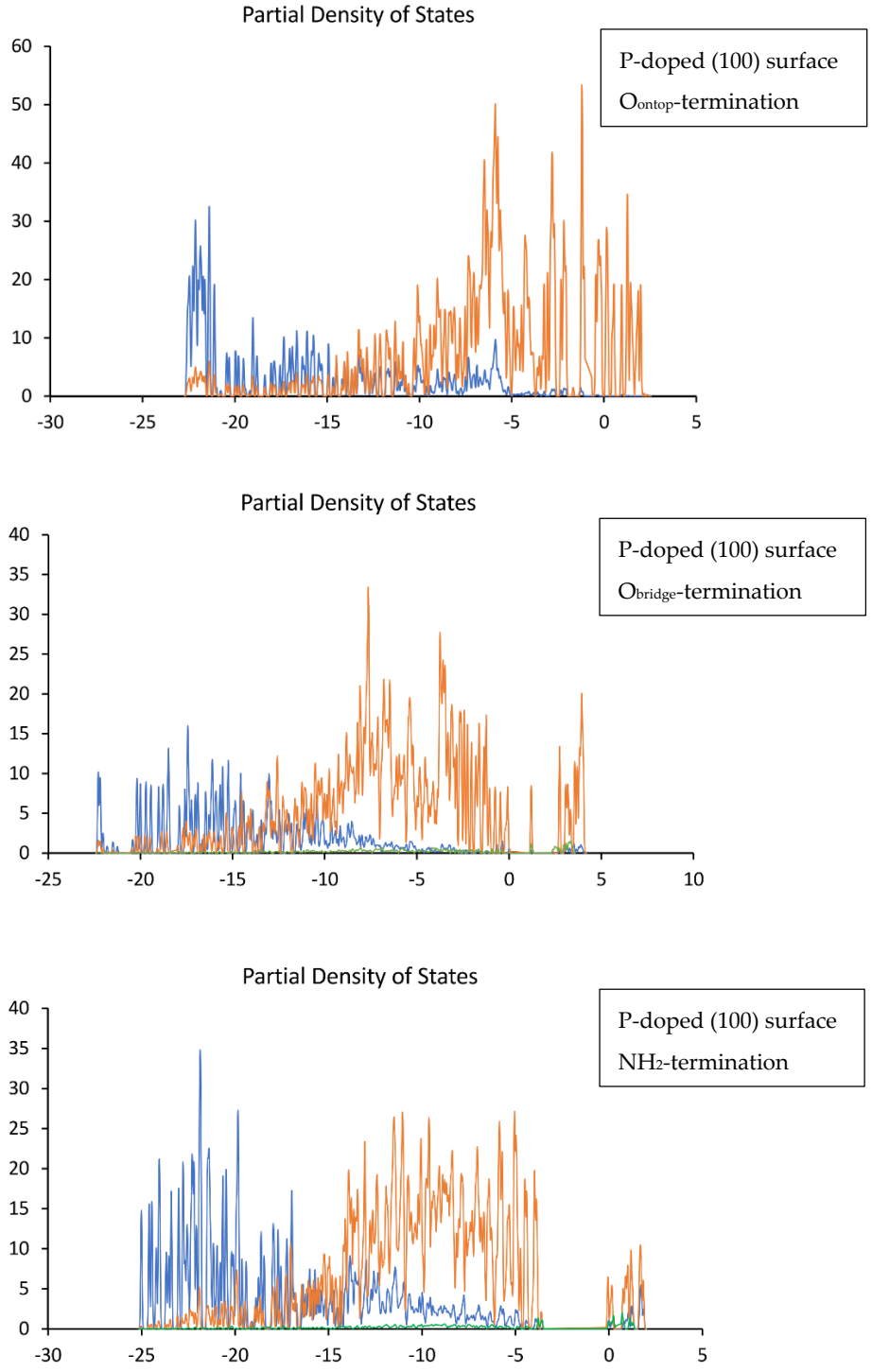

Figure S4. Calculated DOS spectra for P-doped terminated (100) surfaces. The spectra cover the upper surface parts (i.e., terminating layer and C atoms in the upper two atomic layers). The unit of the x-axis is eV, and the unit of the y-axis is electron density. The Fermi level is positioned at 0 eV. Blue: s-states; Orange: p-states.; Green: d-states.

Figure S5

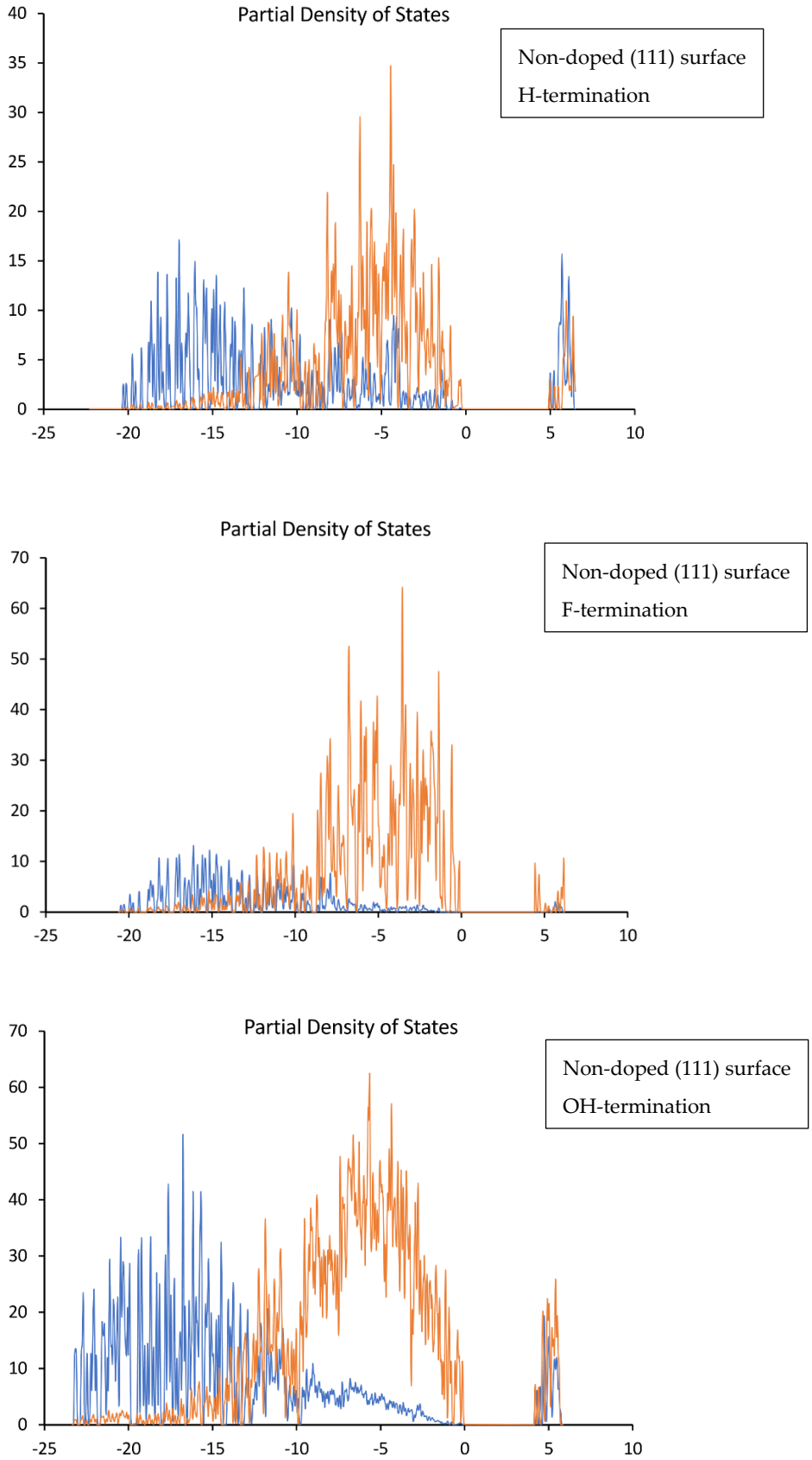
Partial Density of States
Non-doped (111) surface
H-termination
Partial Density of States
Non-doped (111) surface
F-termination
Partial Density of States
Non-doped (111) surface
OH-termination

Figure S5 (cont.)

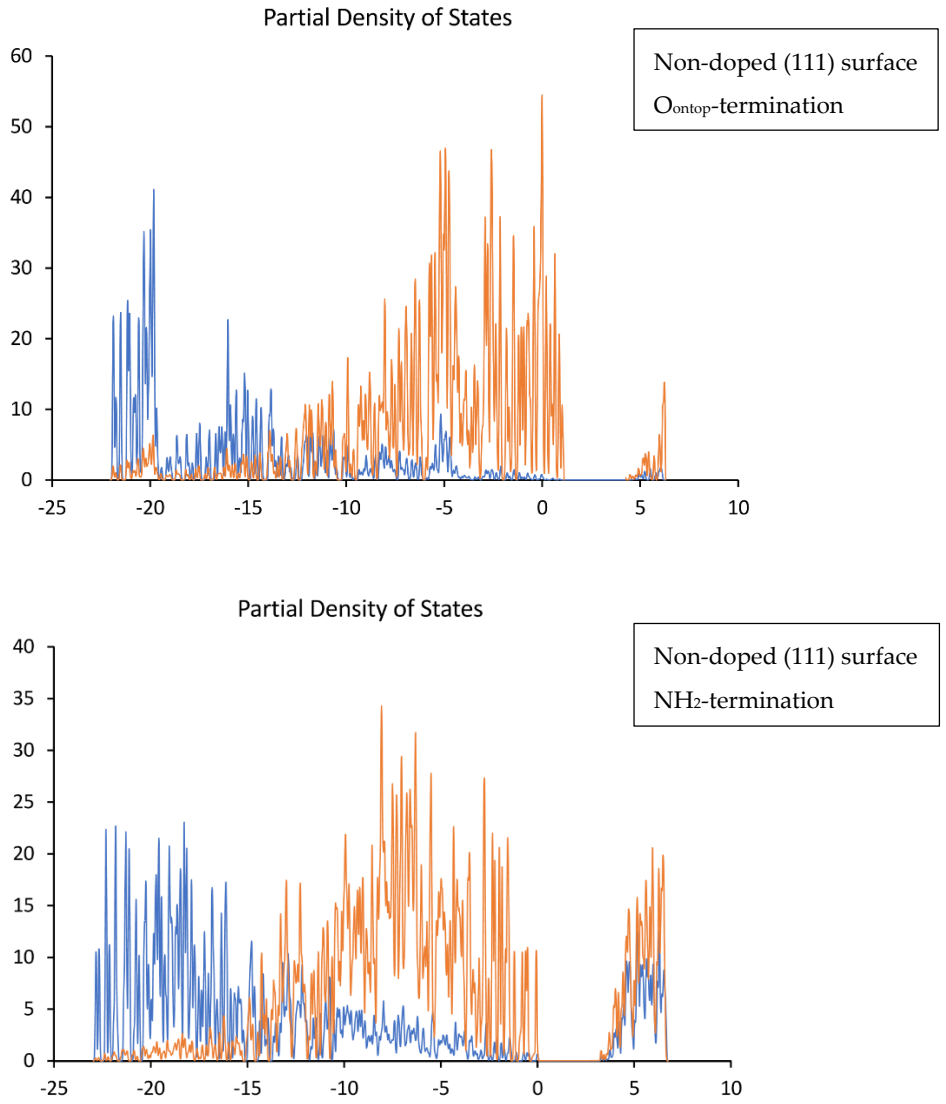

Figure S5. Calculated DOS spectra for non-doped terminated (111) surfaces. The spectra cover the upper surface parts (i.e., terminating layer and C atoms in the upper two atomic layers). The unit of the x-axis is eV, and the unit of the y-axis is electron density. The Fermi level is positioned at 0 eV. Blue: s-states; Orange: p-states.

Figure S6

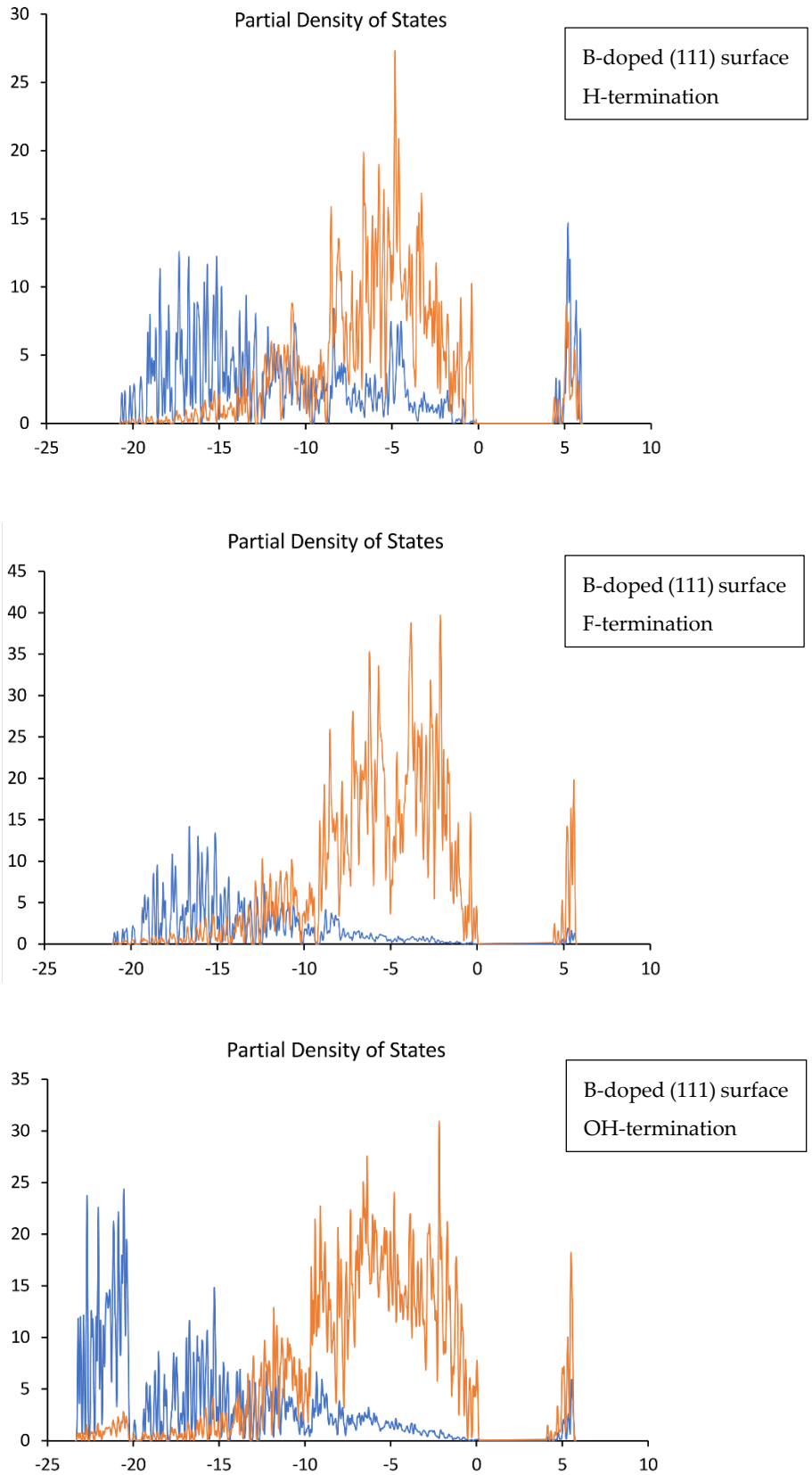
Partial Density of States
B-doped (111) surface
H-termination
Partial Density of States
B-doped (111) surface
F-termination
Partial Density of States
B-doped (111) surface
OH-termination

Figure S6 (cont.)

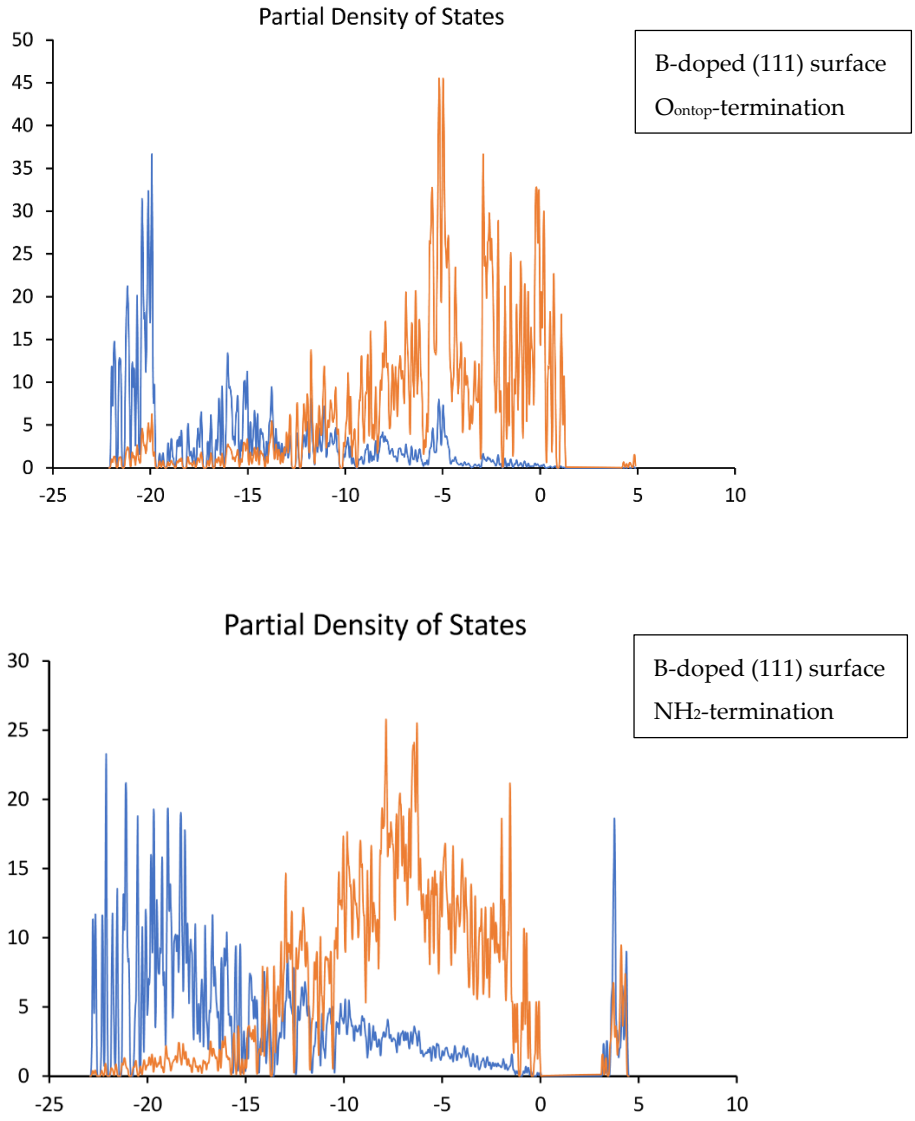

Figure S6. Calculated DOS spectra for B-doped terminated (111) surfaces. The spectra cover the upper surface parts (i.e., terminating layer and C atoms in the upper two atomic layers). The unit of the x-axis is eV, and the unit of the y-axis is electron density. The Fermi level is positioned at 0 eV. Blue: s-states; Orange: p-states.

Figure S7

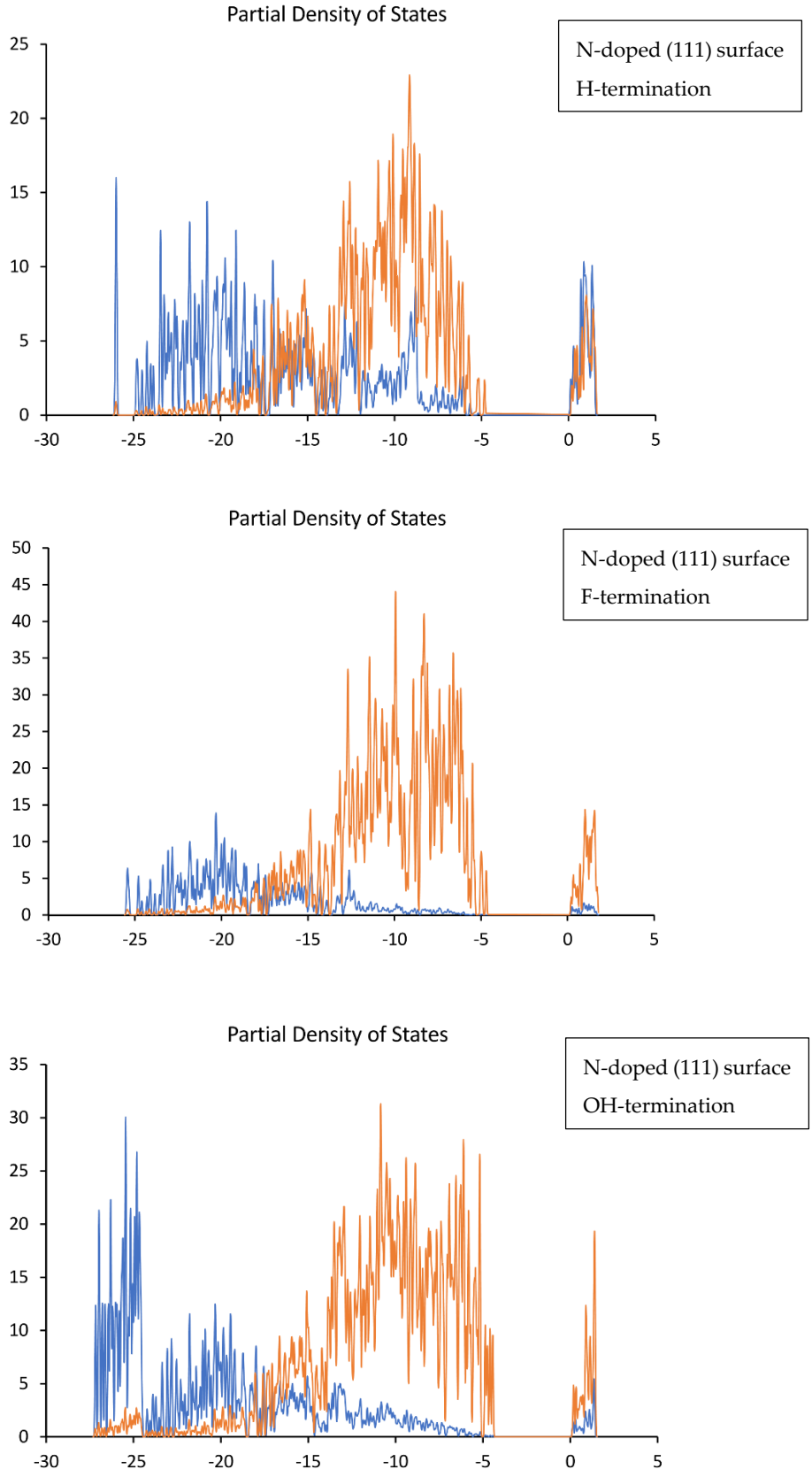
Partial Density of States
N-doped (111) surface
H-termination
Partial Density of States
N-doped (111) surface
F-termination
Partial Density of States
N-doped (111) surface
OH-termination

Figure S7 (cont.)

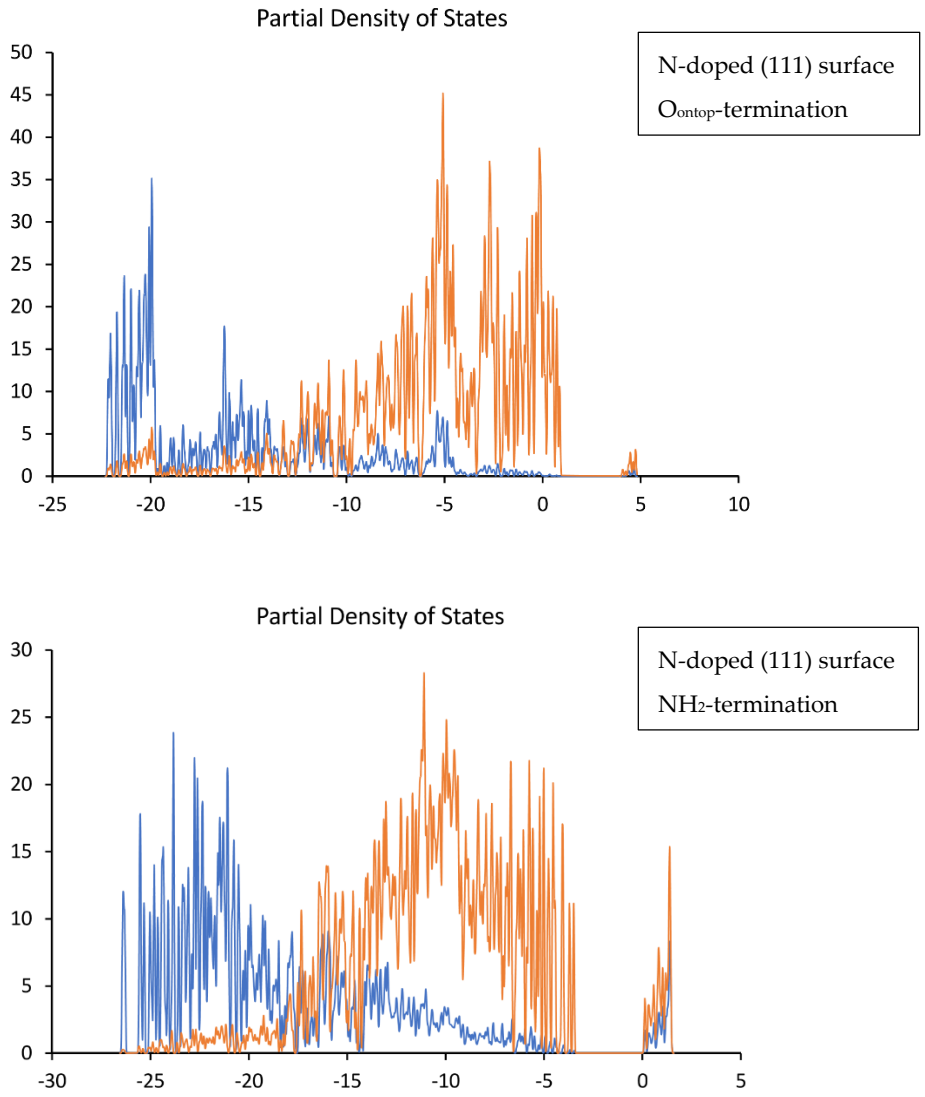

Figure S7. Calculated DOS spectra for N-doped terminated (111) surfaces. The spectra cover the upper surface parts (i.e., terminating layer and C atoms in the upper two atomic layers). The unit of the x-axis is eV, and the unit of the y-axis is electron density. The Fermi level is positioned at 0 eV. Blue: s-states; Orange: p-states.

Figure S8

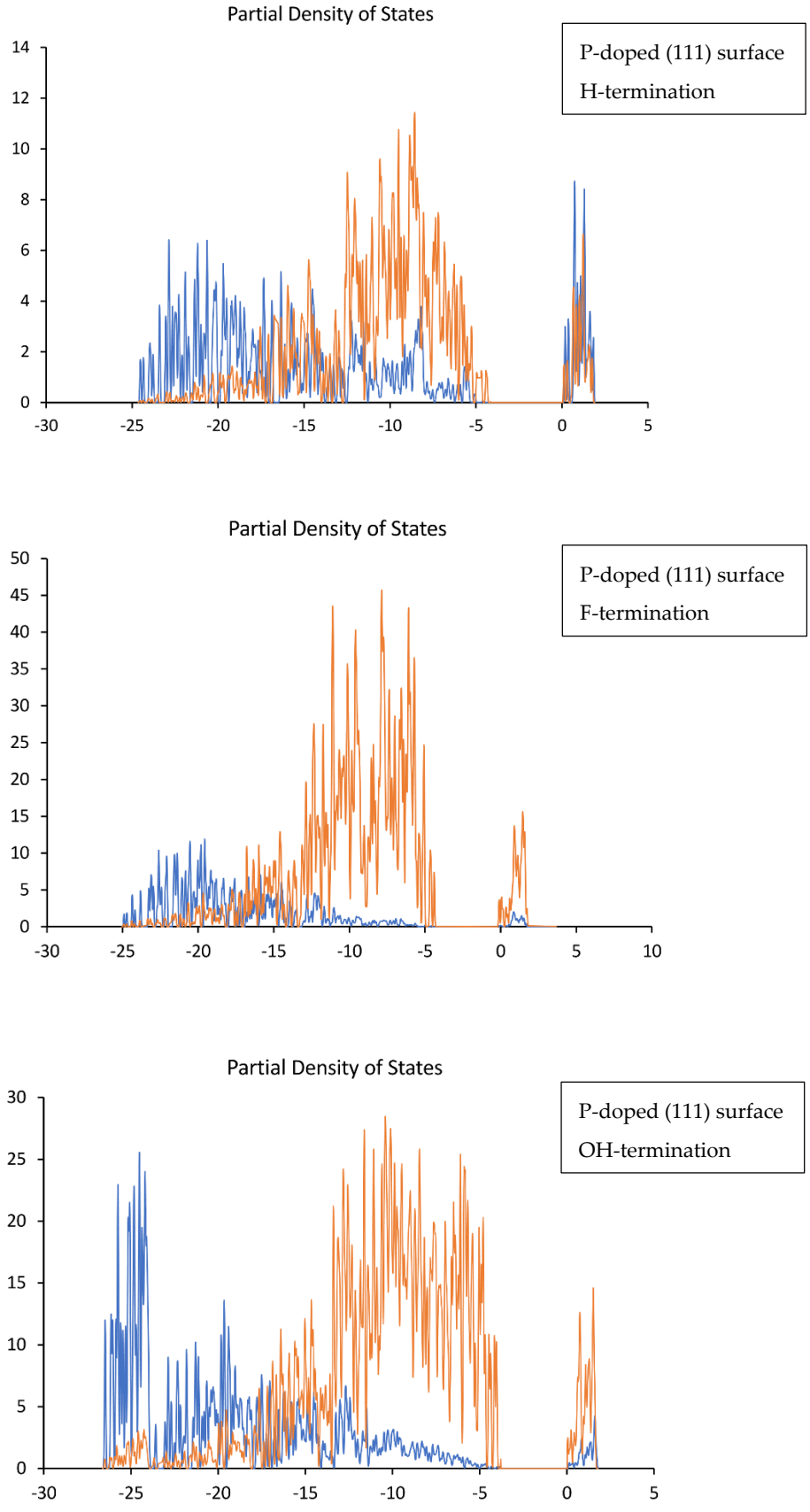
Partial Density of States
P-doped (111) surface
H-termination
Partial Density of States
P-doped (111) surface
F-termination
Partial Density of States
P-doped (111) surface
OH-termination

Figure S8 (cont.)

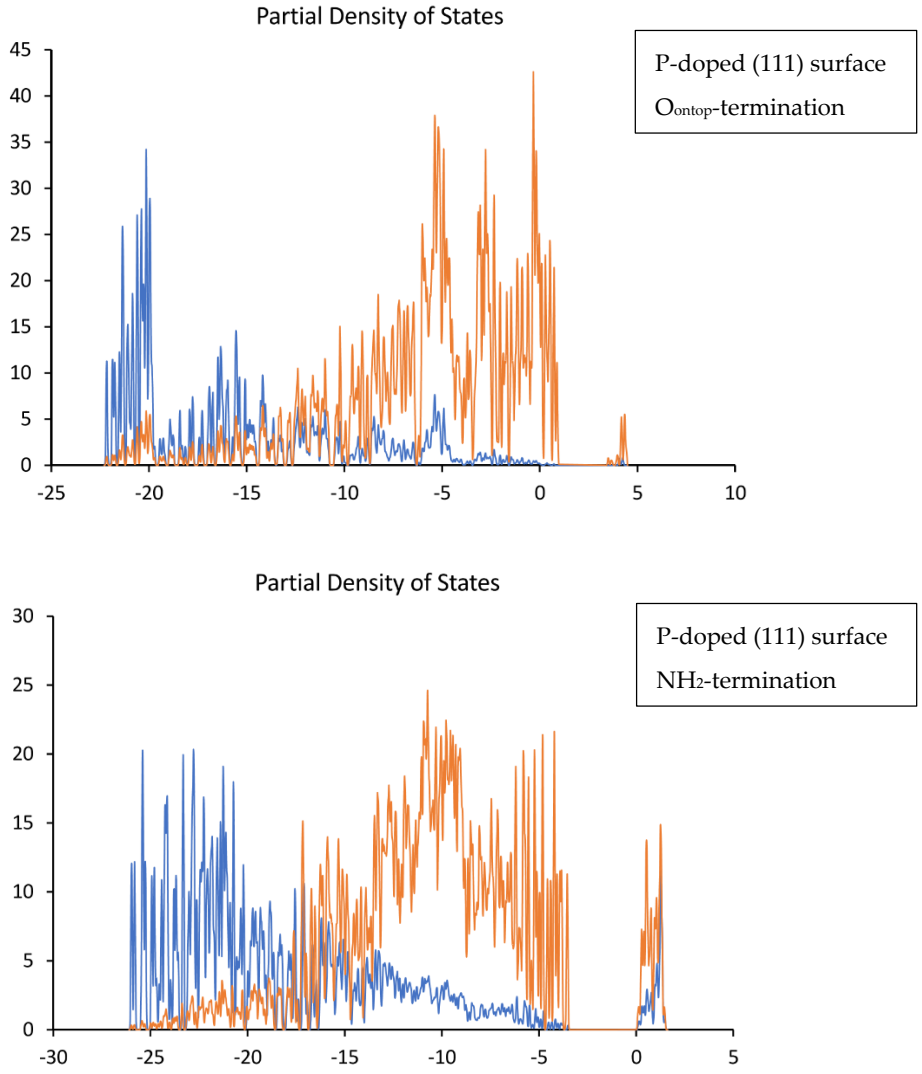

Figure S8. Calculated DOS spectra for P-doped terminated (111) surfaces. The spectra cover the upper surface parts (i.e., terminating layer and C atoms in the upper two atomic layers). The unit of the x-axis is eV, and the unit of the y-axis is electron density. The Fermi level is positioned at 0 eV. Blue: s-states; Orange: p-states.