

Supporting Information for:

The Local Electron Attachment Energy and the Electrostatic Potential as Descriptors of Surface- Adsorbate Interactions

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ADSORPTION FIGURE OPTIMAL SCALES

Figure S1 shows the descriptor map images from Figure 5 of the main article with optimized color scales for the individual particles.

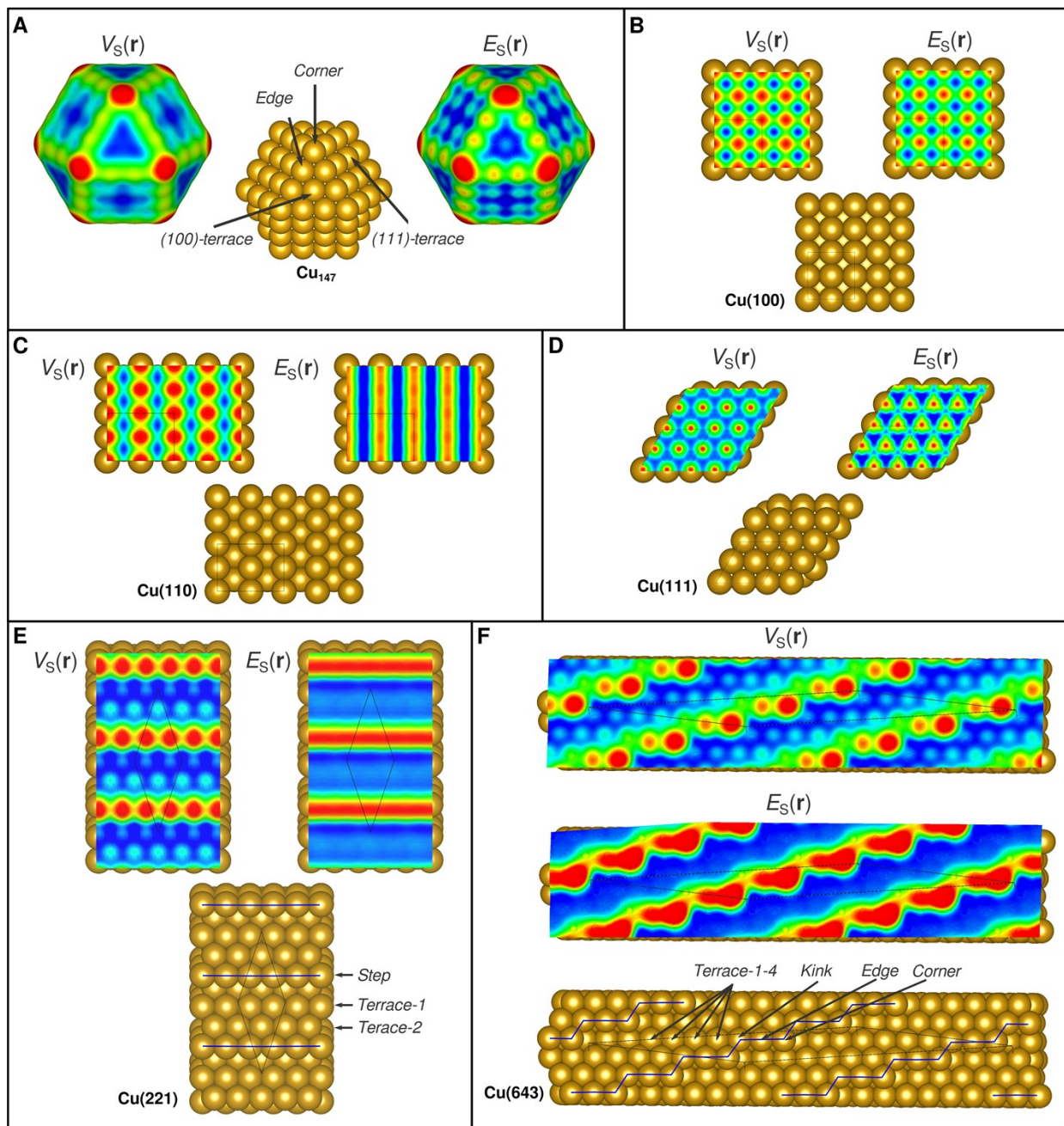


Figure S1. Descriptor map images from Figure 5 of the main article using optimized color scales.

CONVERGENCE TEST

Tables S1-S4 below contains computed $V_{S,\max}$ and $E_{S,\min}$ values for the Cu(100) surface as a function of variation of a number of parameters. These include the number of \mathbf{k} -points, the vacuum distance, the plane-wave cut-off, and the number of Cu layers in the slab. The standard set-up used for the parameters that are not varied are: 11x11x1 \mathbf{k} -points, 800 eV plane-wave cut-off, 40 Å slab vacuum, and a slab thickness of 10 Cu layers.

In conclusion we can note that $V_{S,\max}$ is very robust to the parameter variations and differs significantly from the converged value only for the most crude parameter choices. $E_{S,\min}$ varies more, but is converged at the set-ups used in the main text. Further tests will be conducted in future studies.

Table S1. K-point test.

k-points	$E_{S,\min}$ (eV)	$V_{S,\max}$ (eV)
15×15×1	-7.73	0.34
13×13×1	-7.73	0.34
11×11×1	-7.73	0.34
9×9×1	-7.78	0.34
8×8×1	-7.82	0.34
6×6×1	-7.84	0.34
4×4×1	-7.86	0.34
2×2×1	-7.78	0.35
1×1×1	-8.46	0.36

Table S2. Vacuum test.

Vacuum (\AA)	$E_{S,\min}$ (eV)	$V_{S,\max}$ (eV)
60	-7.73	0.34
50	-7.73	0.34
40	-7.73	0.34
30	-7.57	0.35
20	-7.30	0.33
15	-7.28	0.34
10	-7.25	0.33

Table S3. Slab thickness test.

Thickness (layers)	$E_{S,\min}$ (eV)	$V_{S,\max}$ (eV)
14	-7.73	0.34
12	-7.73	0.34
10	-7.73	0.34
9	-7.72	0.34
8	-7.68	0.34
6	-7.56	0.33
4 ^a	-7.49	0.33
2 ^a	-6.96	0.33

^a Note that for these structures the full slab was allowed to relax without constraints.

Table S4. Plane-wave cut-off test.

k-points	$E_{S,\min}$ (eV)	$V_{S,\max}$ (eV)
800	-7.73	0.34
700	-7.74	0.34
600	-7.75	0.34
500	-7.75	0.34
400	-7.75	0.34
300	-8.56	0.51