

Bulk (in)stability as a possible source or surface reconstruction

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Table. S1. Influence of the plane-wave kinetic energy cutoff and vacuum width on the surface energy for a (2×2) MoC supercell surface model containing four atomic layers. All surface energy values are in J/m².

Plane Wave kinetic energy Cutoff	415 eV	500 eV
Relaxed surface energy	0.67	0.67
Fixed surface energy	1.41	1.41
Vacuum width	15 Å	20 Å
kinetickiRelaxed surface energy	0.67	0.67
Fixed surface energy	1.41	1.41

Table. S2. Influence of the slab model thickness on the surface energy. Calculations are reported for two (2×2) supercell models, one with 4 atomic layers (2 relaxed + 2 frozen) and one with 8 atomic layers (6 relaxed + 2 frozen). All surface energy values are in J/m².

Thickness	4 layers (2+2)	8 layers (2+6)
Fixed surface energy	1.41	1.44
Relaxed surface energy	0.67	0.48

Figure S1. Initial configurations of the alternative reconstruction patterns studied in the (4×4) supercell of MoC (001) surface. Purple and black spheres correspond to Mo and C atoms, respectively. Atoms displacements are shown by arrows.

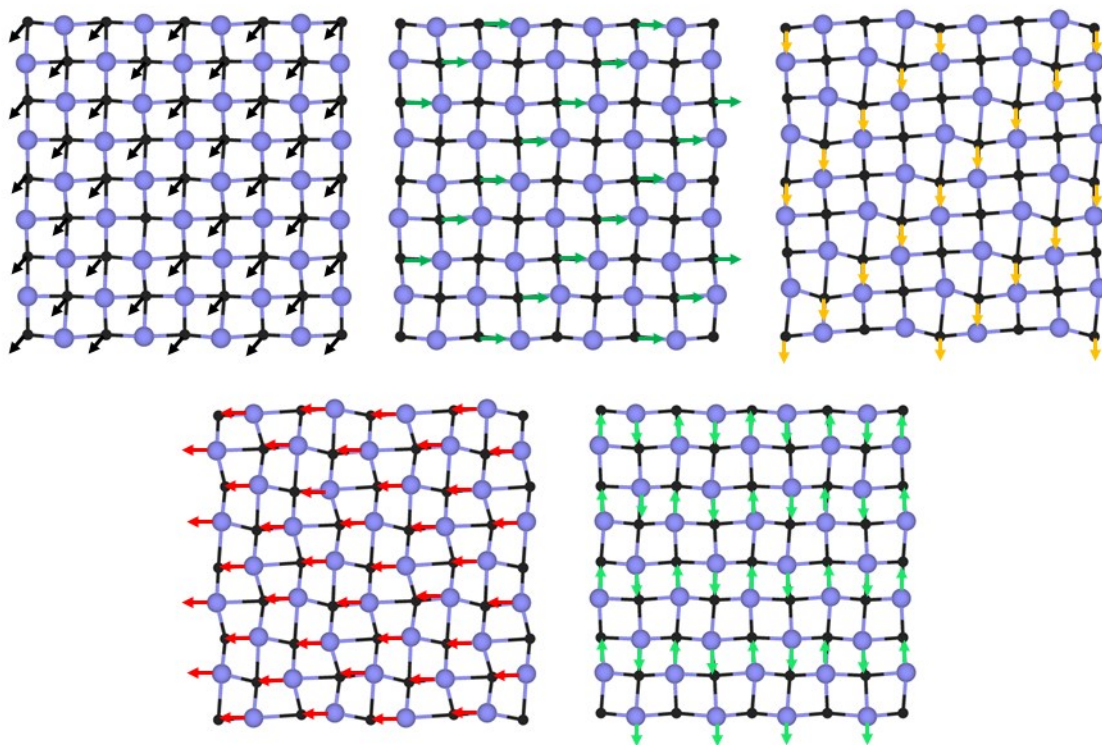


Figure. S2. First (top panels) and second (bottom panels) atomic layer for fixed (bulk-truncated) vs. reconstructed (2×2) supercells of the MoN (001) surface. Violet and cyan spheres correspond to Mo and N atoms, respectively.

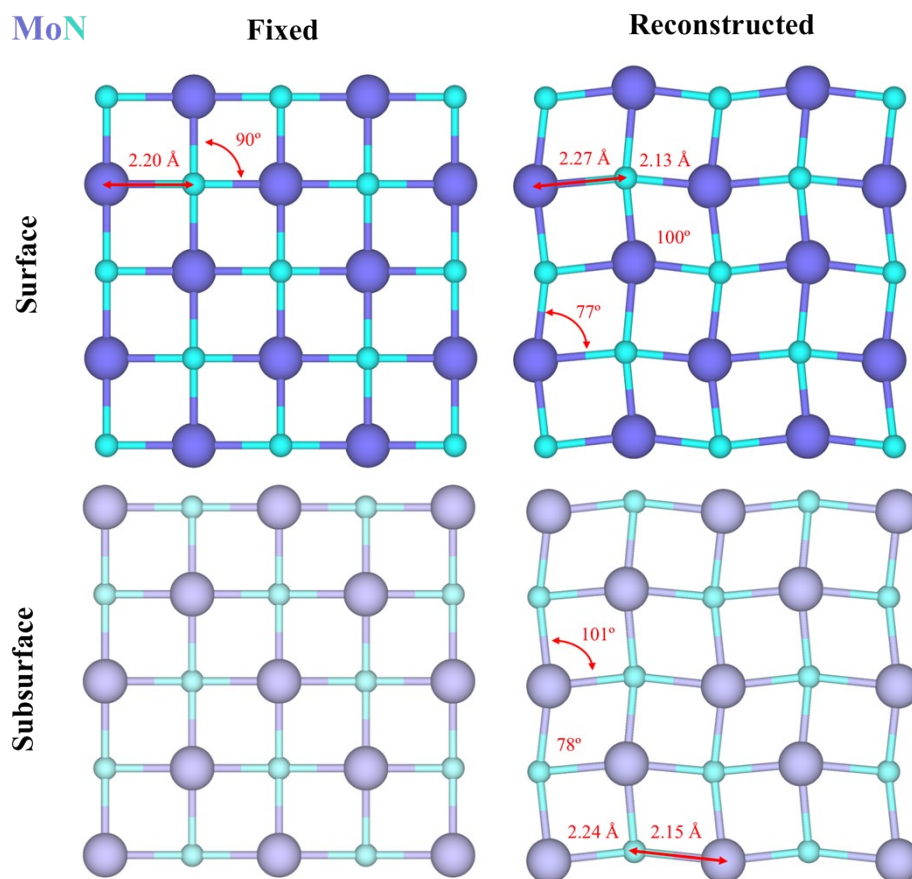


Figure S3. First (top panels) and second (bottom panels) atomic layer for fixed (bulk-truncated) vs. reconstructed (2×2) supercells of the γ -WC (001) surface. Grey and black spheres correspond to W and C atoms, respectively.

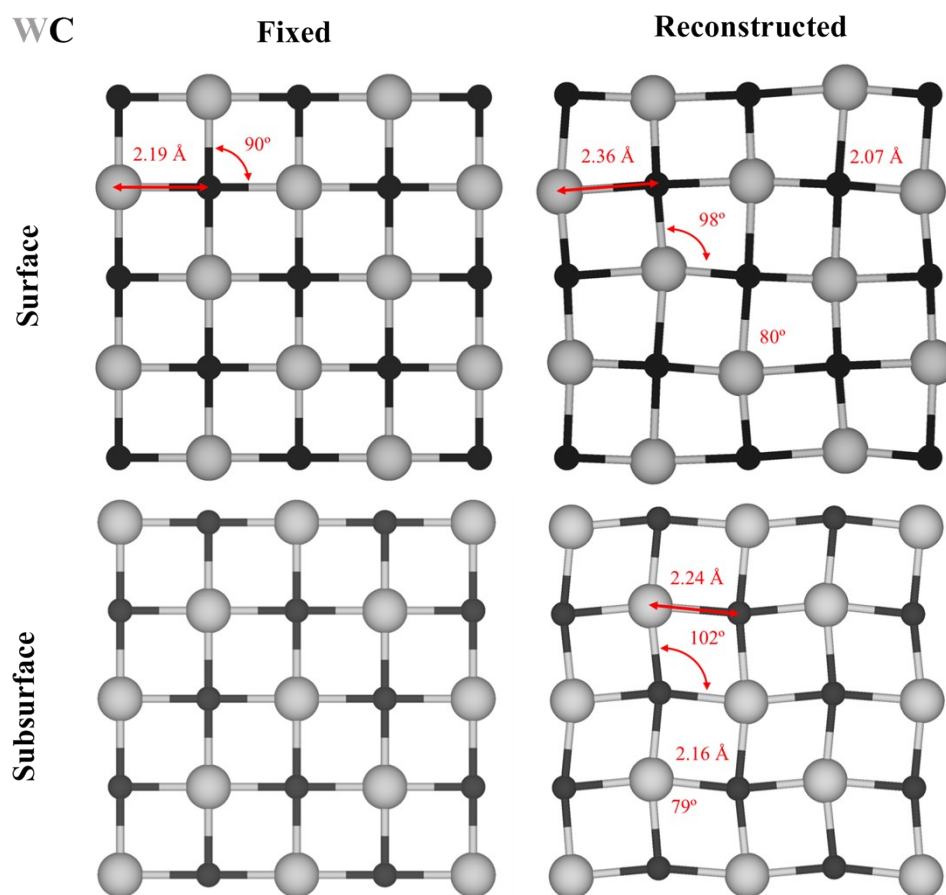


Figure S4. First (top panels) and second (bottom panels) atomic layer for fixed (bulk-truncated) vs. reconstructed (2×2) supercells of the WN (001) surface. Grey and cyan spheres correspond to W and N atoms, respectively.

