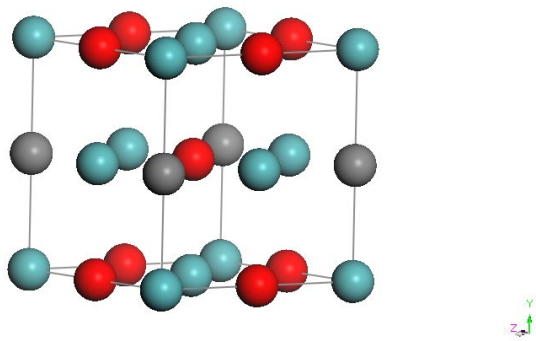
## Supporting Information Content:

Calculated model cell parameters for the MoOC system, and HRTEM simulated images for MoO fcc model:



Red, Blue and gray correspond to Oxygen, Molybdenum and Carbon.

Lattice parameters(A) Cell Angles

a =4.331726 alpha =89.999993

b =4.331701 beta =89.999939

c =4.331702 gamma =89.999969

Current cell volume =81.278941 $A^3$

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Cell Contents

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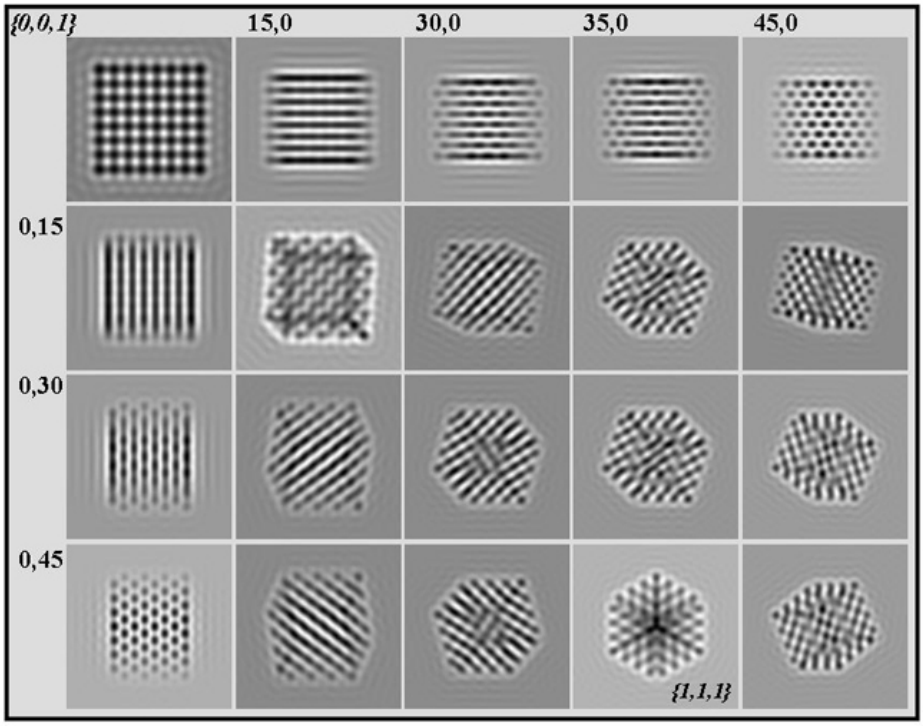
Total number of ions in cell = 8

Total number of species in cell = 3

Max number of any one species = 4

| Element | Atom Number | Fractional coordinates of atoms | | |
|---|---|---|---|---|
| | | u | v | w |
| C | 1 | 0.000000 | 0.499999 | 0.000000 |
| O | 1 | 0.500001 | 0.000000 | 0.000000 |
| O | 2 | 0.500001 | 0.500002 | 0.500001 |
| O | 3 | 0.000000 | 0.000000 | 0.500001 |
| Mo | 1 | 0.000000 | 0.000000 | 0.000000 |
| Mo | 2 | 0.000000 | 0.500000 | 0.499999 |
| Mo | 3 | 0.499999 | 0.000000 | 0.499999 |
| Mo | 4 | 0.499999 | 0.500000 | 0.000000 |




HRTEM simulated images for MoO fcc model for each 15$^{o}$ and the 35$^{o}$ up to reach the {1,1,1}.