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Structures and Thermodynamic Stability of Cobalt Molybdenum Oxide (CoMoO₄-II)

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Highlights

- Estimated properties of bulk CoMoO_4 -II reproduce limited analogous experimental measurements.
- Upward displacement of surface oxygen atoms is observed in most optimized surfaces.
- Mo/Co-O bonds display an ionic character.
- O-truncated surfaces dominate the thermodynamic stability trend.

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