



Supporting Information

for

Improvement of the thermoelectric properties of a MoO₃ monolayer through oxygen vacancies

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Beilstein J. Nanotechnol. **2019**, *10*, 2031–2038. doi:10.3762/bjnano.10.199

Crystal structures of MoO₃ with oxygen vacancies

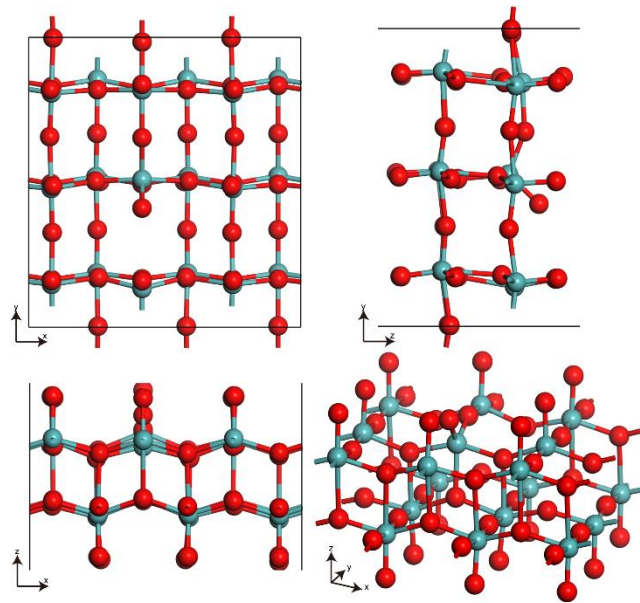


Figure S1: Optimized structure of MoO₃ monolayer with O1 vacancy. The red spheres represent O atoms and the green represent Mo atoms.

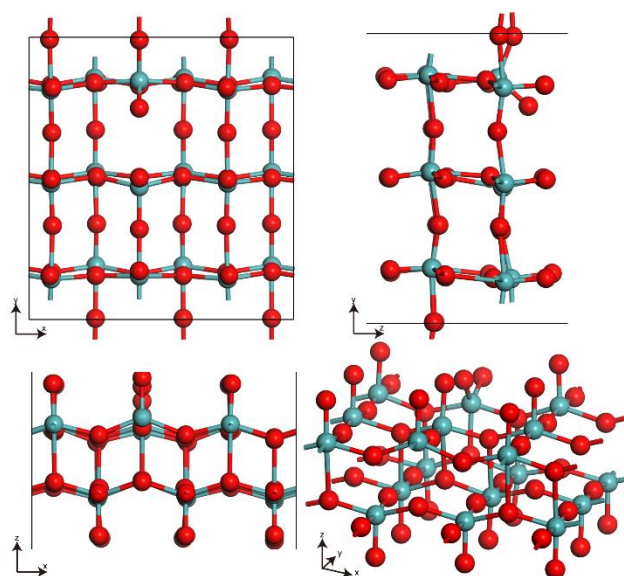


Figure S2: Optimized structure of MoO₃ monolayer with O₂ vacancy. The red spheres represent O atoms and the green represent Mo atoms.

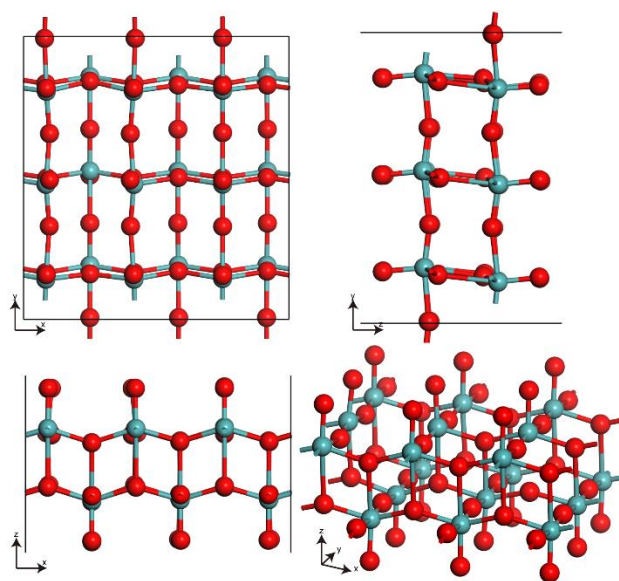


Figure S3: Optimized structure of MoO₃ monolayer with O₃ vacancy. The red spheres represent O atoms and the green represent Mo atoms.