

Supporting Information

A van der Waals Density Functional Study of MoO₃ and its Oxygen Vacancies

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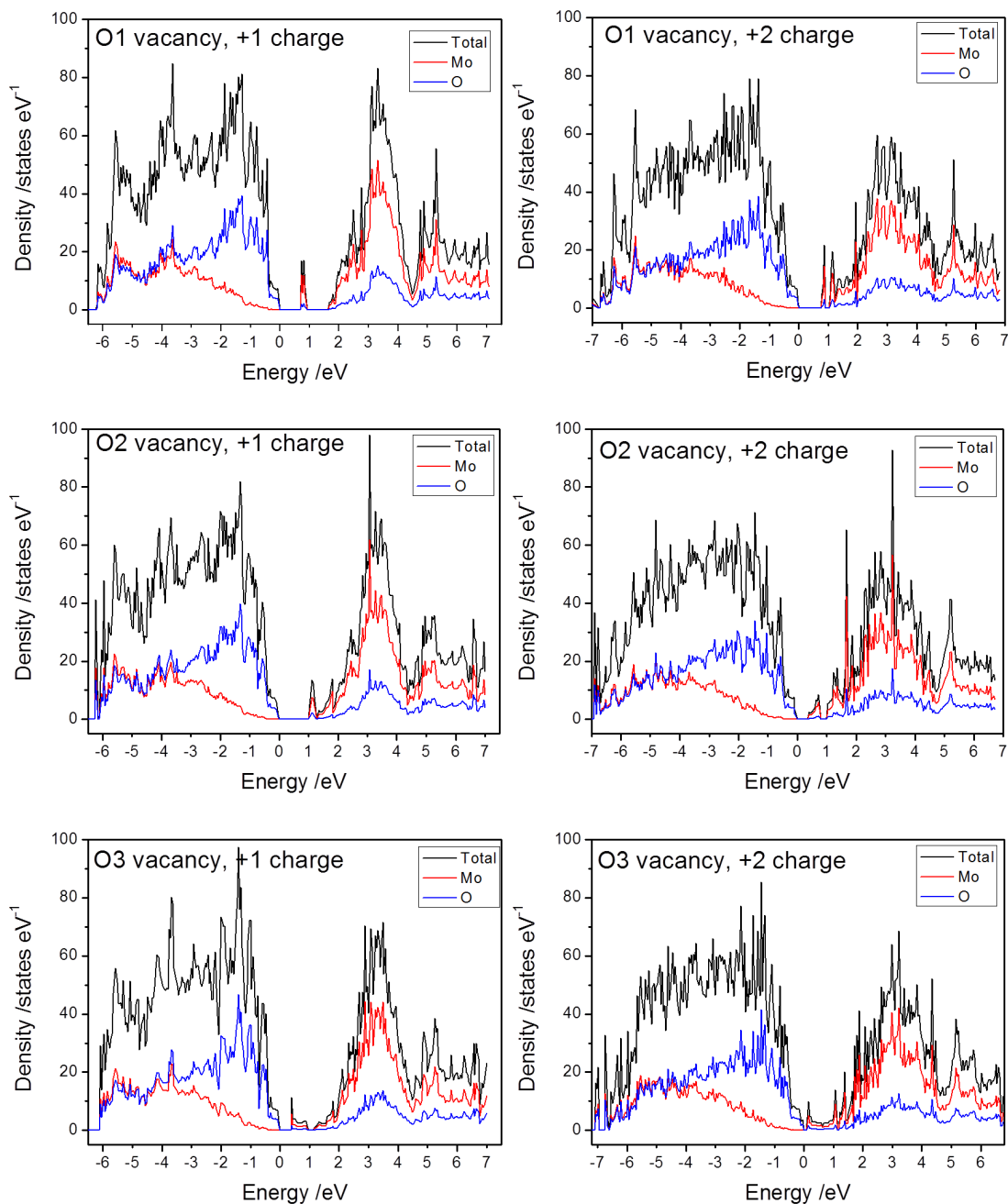


Figure S1. Total and partial density of states of oxygen vacancies on the three oxygen positions with +1 and +2 charges.

The density of states for charged cells shows reduction of the band gap of MoO₃ with increasing charge. There is also further dispersion of the gap states compared to neutral cells due to the effect of the U parameter on unoccupied states.