

Theoretical study of SF₆ adsorption and decomposition over the MgO (001) and (111) surfaces

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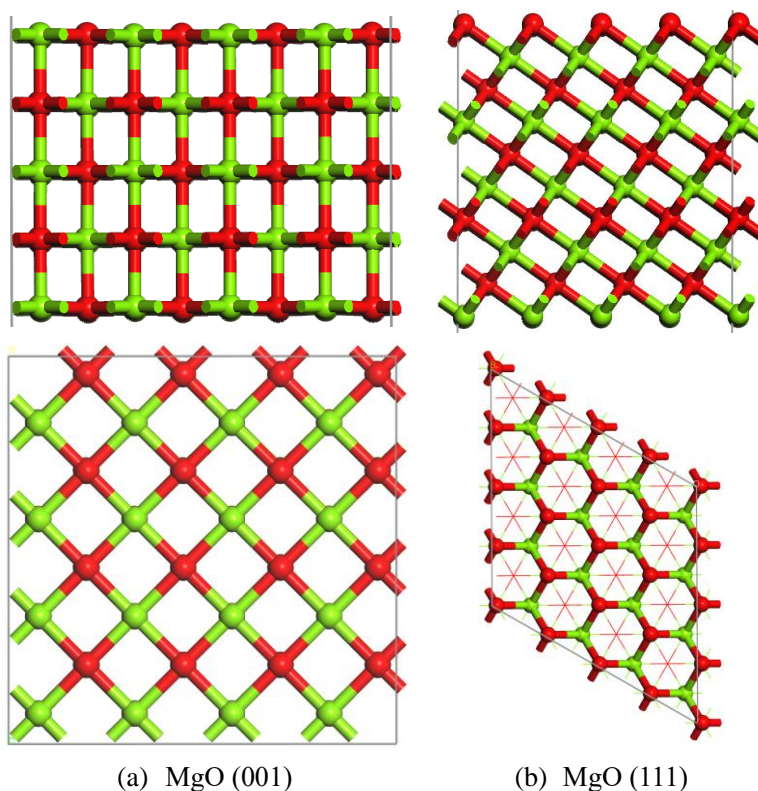


Fig.S1 Bulk models of the perfect MgO (001) (a) and O-terminated (111) (b) slabs, in side view (upper panels) and top view (lower panels). Green and red balls are Mg and O atoms, respectively.

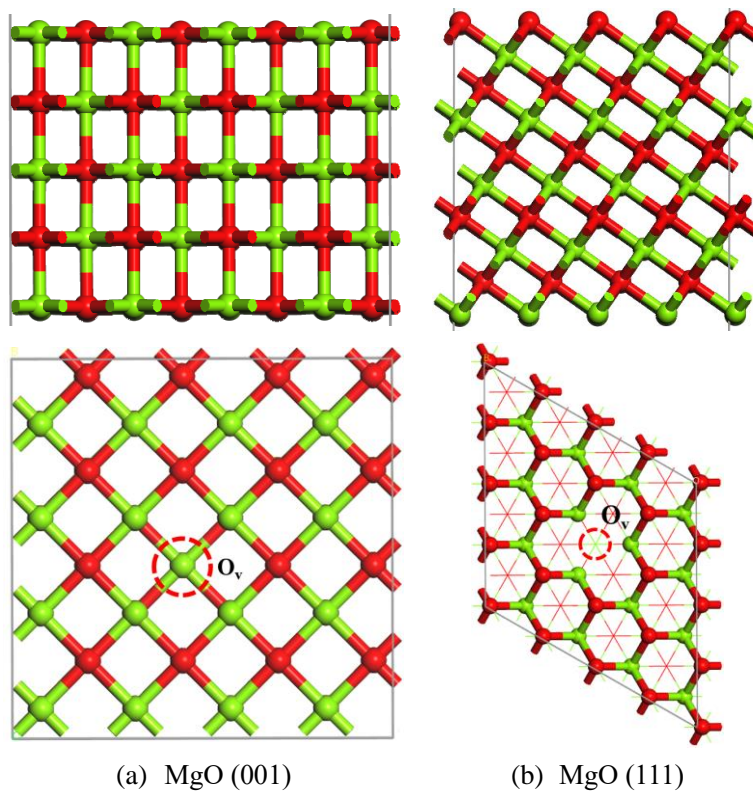
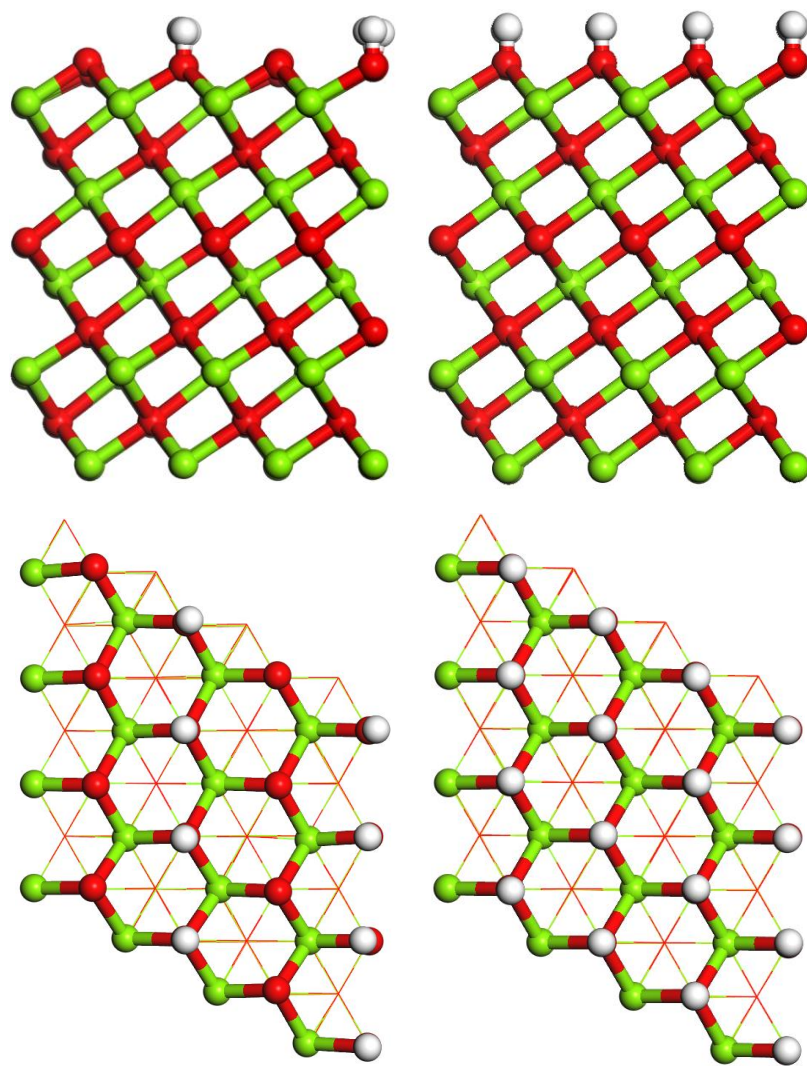


Fig.S2 Bulk models of the MgO (001) (a) and O-terminated (111) slabs (b) with one O vacancy (O_v), in side view (upper panels) and top view (lower panels). Green and red balls are Mg and O atoms, respectively.



(a) 0.5 ML

(b) 1.0 ML

Fig.S3 Bulk models of the O-terminated (111) slabs with 0.5 (a) and 1.0 ML (b) H-coverage, in side view (upper panels) and top view (lower panels). Green, red and white balls are Mg, O and H atoms, respectively.