Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Generation of highly reactive oxygen species on metal-supported MgO(100) thin films

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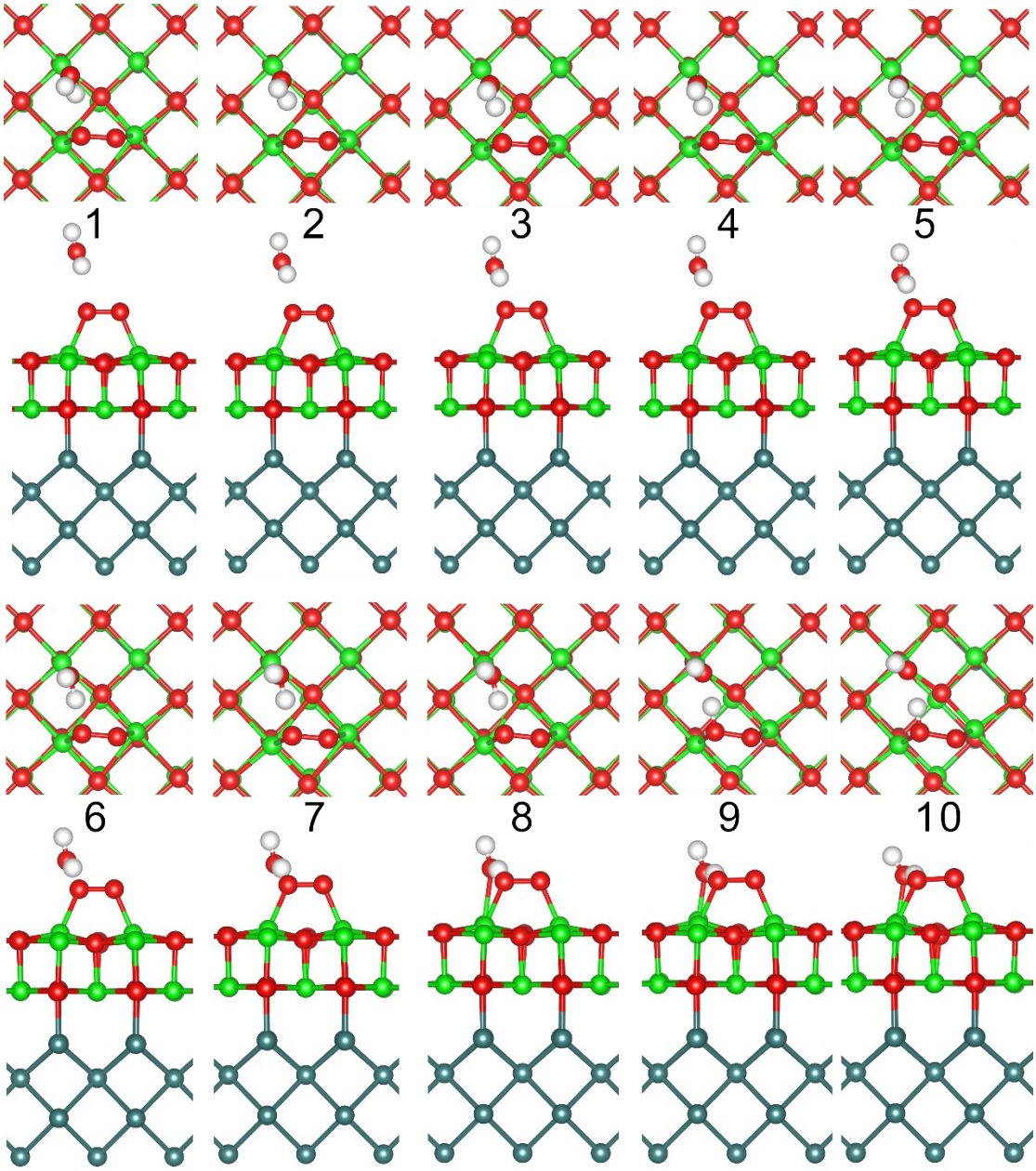

Fig. S1. Geometrical configurations for the image points of OOH formation pathway on 2 ML MgO(100)/Mo(100) shown in Fig. 4. The Arabic numerals 1-10 label all relevant reaction steps.

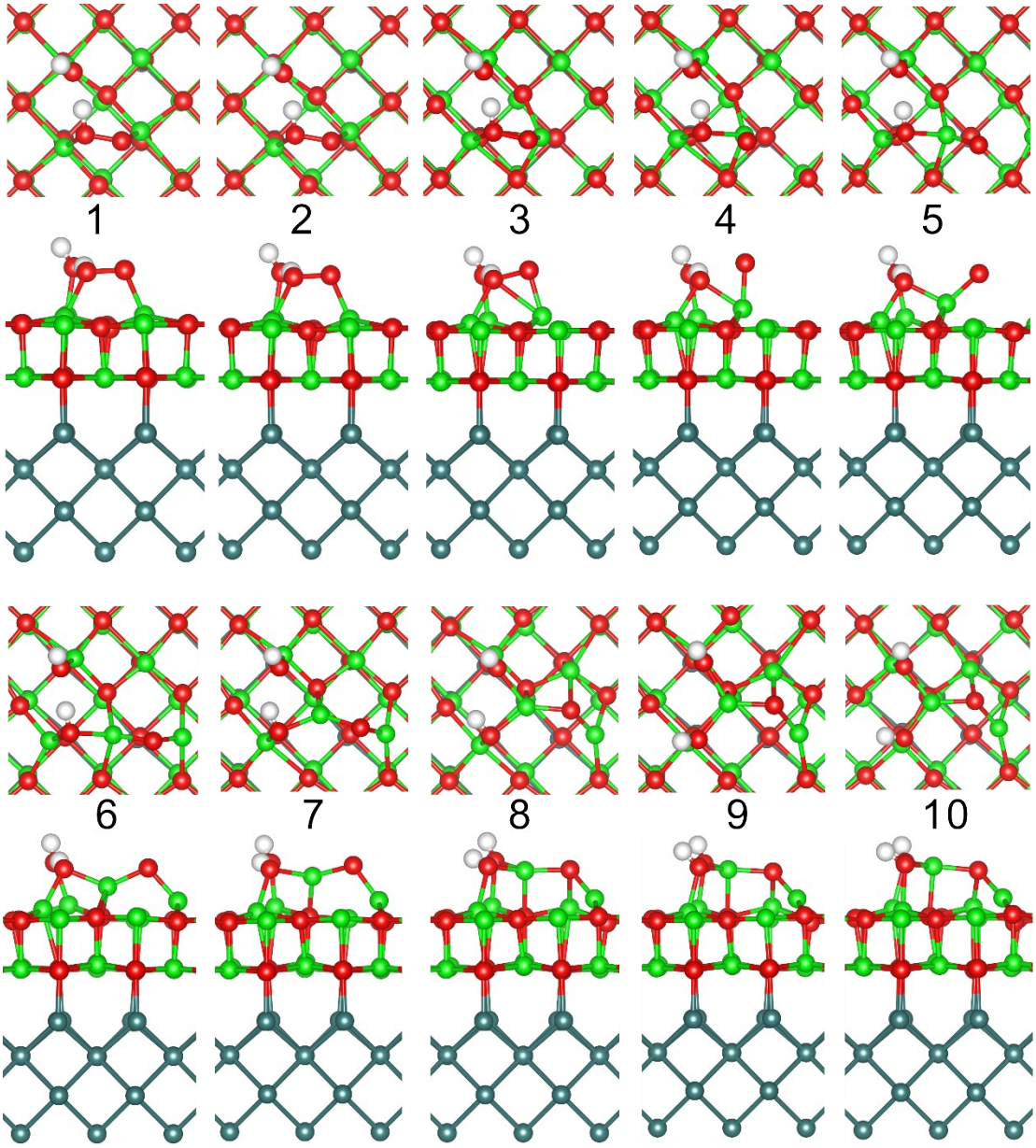

Fig. S2. Geometrical configurations for the image points of producing high reactive oxygen adatom and hydroxyl species on 2 ML MgO/Mo(100) surface shown in Fig. 5. The Arabic numerals 1-10 label all relevant reaction steps..

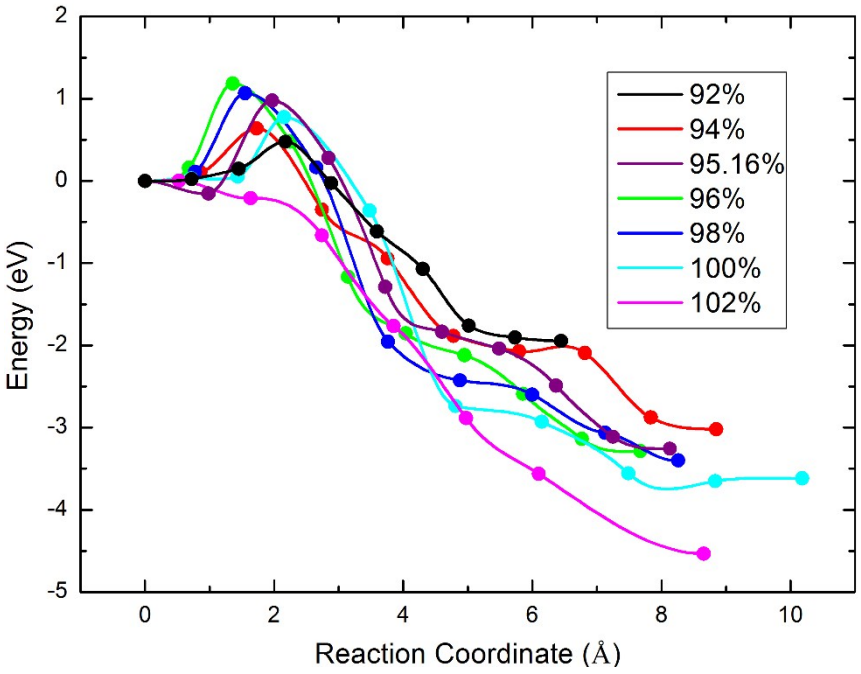

Fig. S3. Potential energy profiles for OOH splitting to produce OH and oxygen adatom on 2 ML MgO/Mo(100) surfaces with various lattice constants of Mo substrate. The corresponding lattice mismatches between MgO film and Mo substrate is in the range from-3.3% to 7.2%.

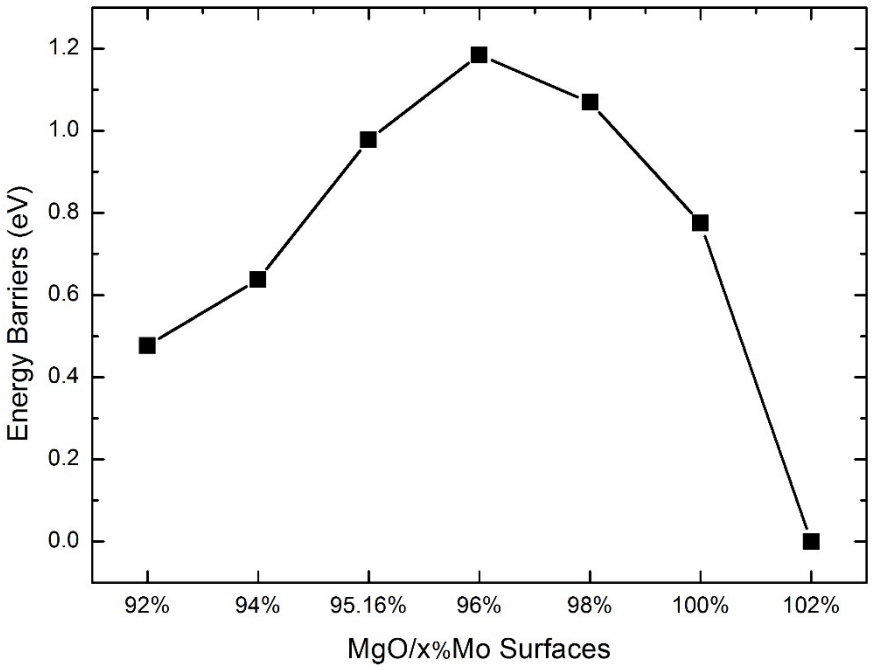

Fig. S4. The relationship between energy barriers and lattice constants of Mo substrate for the splitting of OOH.