

Mechanism of Coverage Dependent CO Adsorption and Dissociation on the Mo(100) Surface

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Content

Fig. S1-S10 All calculated transition state structures for CO dissociation at all coverage

Fig. S1: Structures of 1CO dissociation on Mo(100) surface.

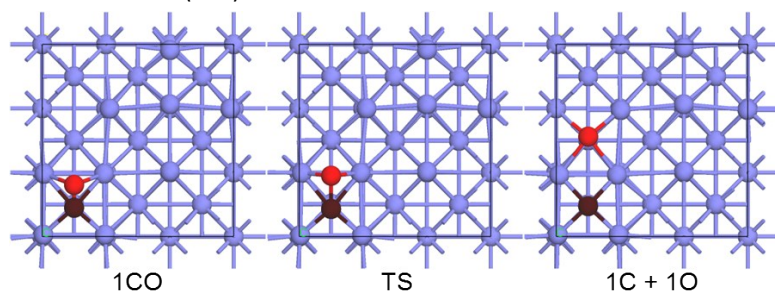


Fig. S2: Structures of 2CO dissociation on Mo(100) surface.

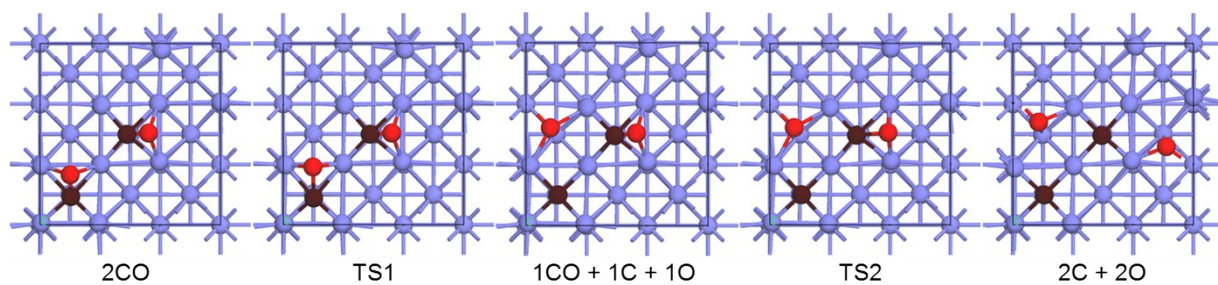


Fig. S3: Structures of 3CO dissociation on Mo(100) surface.

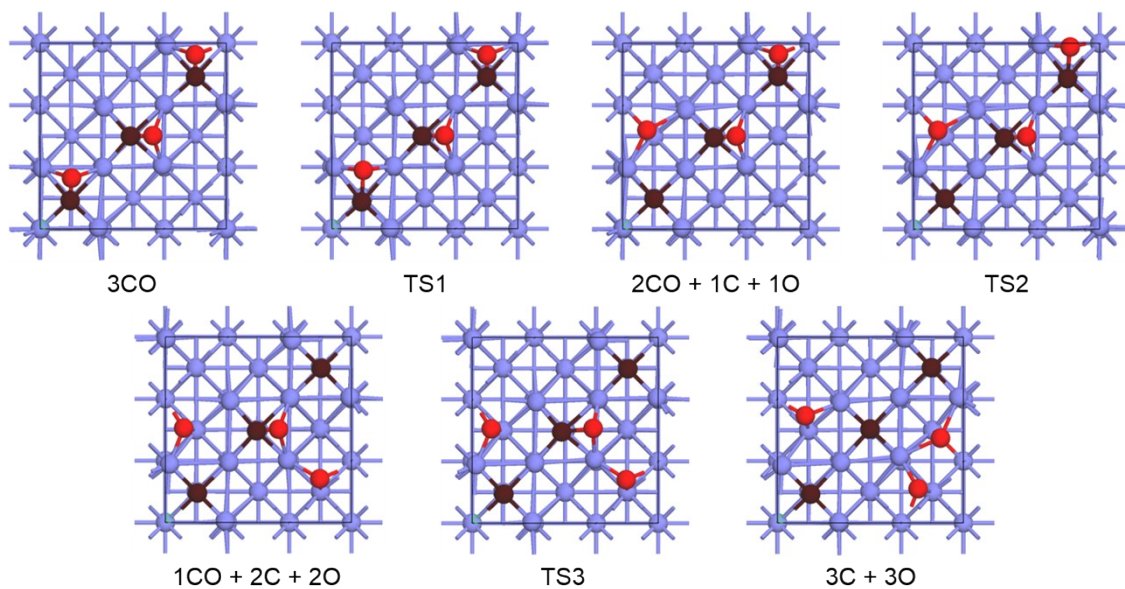


Figure S4: Structures of 4CO dissociation on Mo(100) surface.

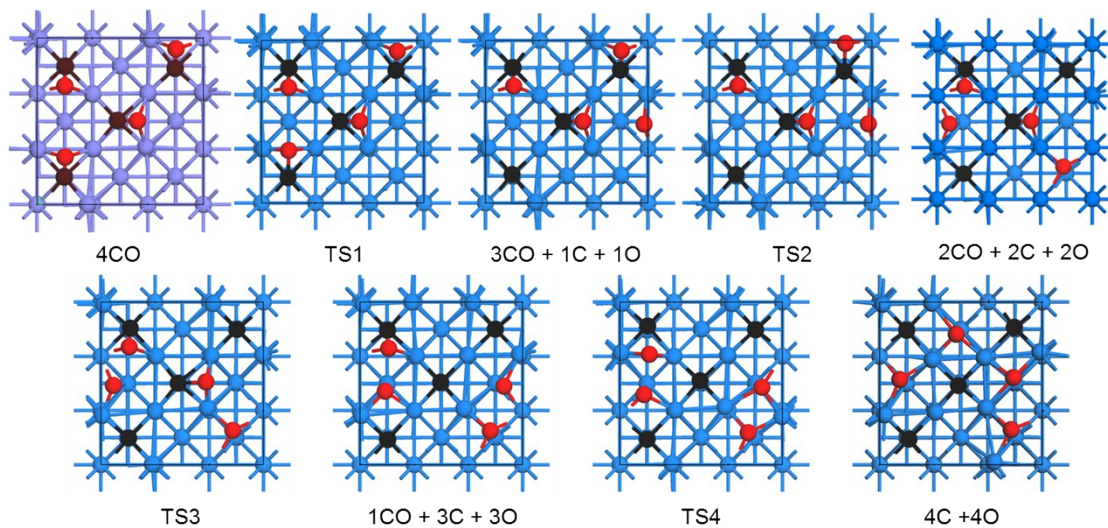


Figure S5: Structures of 5CO dissociation on Mo(100) surface.

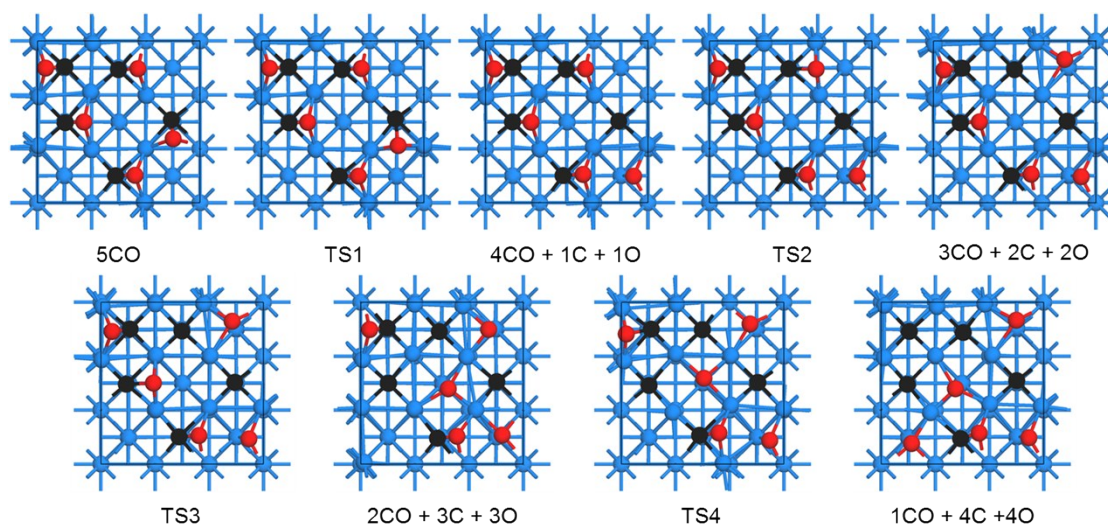


Figure S6: Structures of 6CO dissociation on Mo(100) surface.

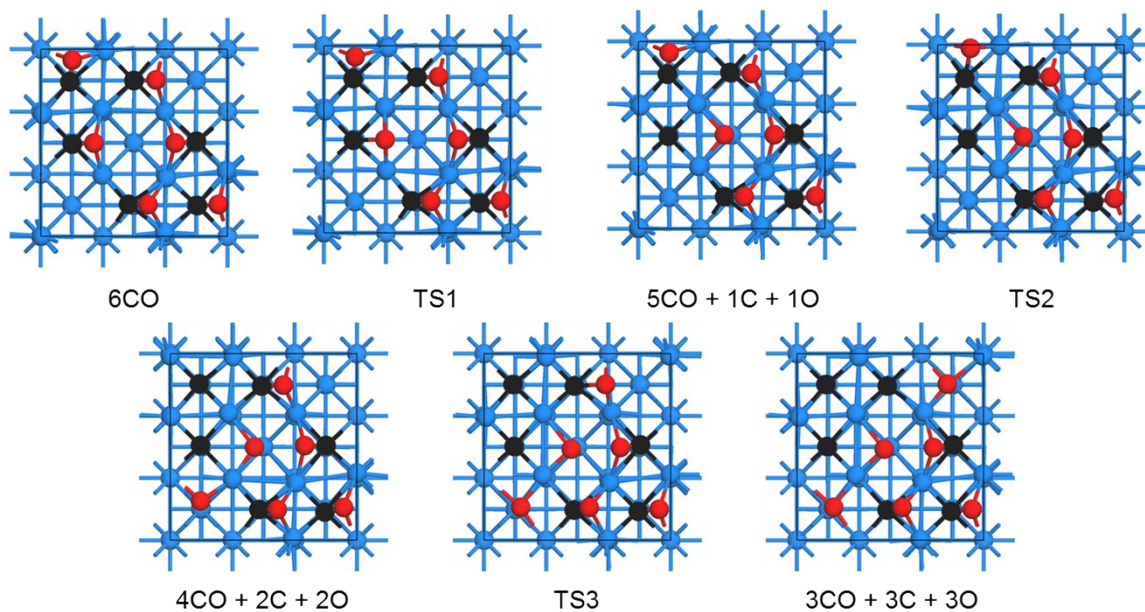


Figure S7: Structures of 7CO dissociation on Mo(100) surface.

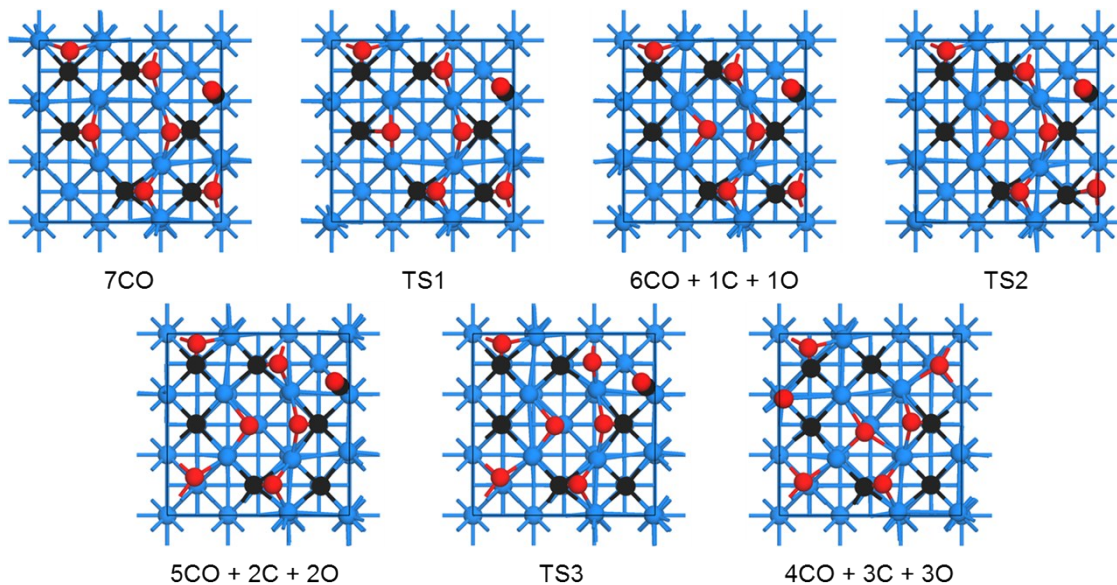


Fig. S8: Structures of 8CO dissociation on Mo(100) surface.

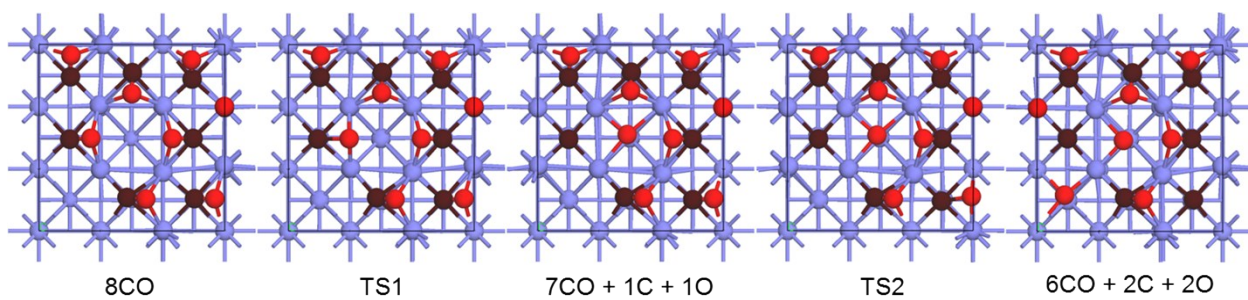


Fig. S9: Structures of 9CO dissociation on Mo(100) surface.

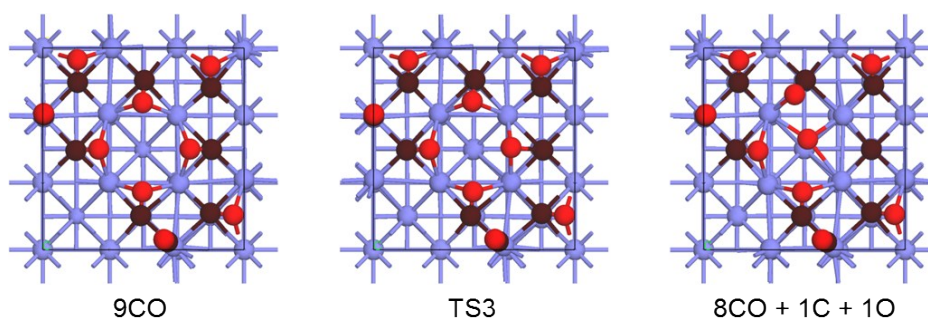


Fig. S10: Structures of 10CO dissociation on Mo(100) surface.

