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

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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.

6CO  
TS1  
5CO + 1C + 1O  
TS2  
4CO + 2C + 2O  
TS3  
3CO + 3C + 3O

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

7CO  
TS1  
6CO + 1C + 1O  
TS2  
5CO + 2C + 2O  
TS3  
4CO + 3C + 3O

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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.