

Ru-catalyzed steam methane reforming: Mechanistic study from first principles calculations

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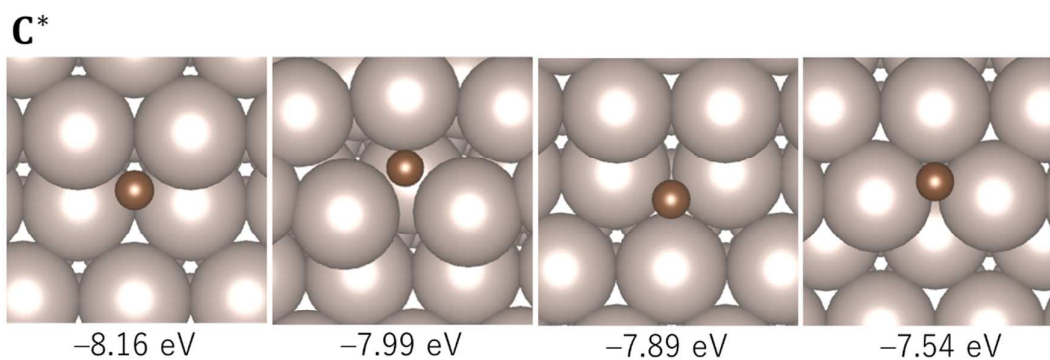
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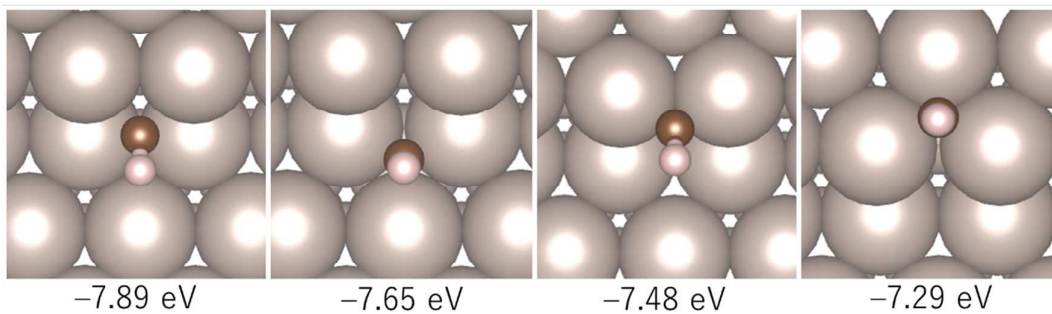
Table S1: Adsorption energies

Adsorbed species	Adsorption energies (eV)
C	-8.16076
CH	-7.88902
CH ₂	-4.85246
CH ₃	-3.09906
CH ₄	-0.3929
CO	-2.41012
COH	-5.15204
CHO	-3.57508
CHOH	-3.06315
CH ₂ O	-2.01807
CH ₂ OH	-2.9814
CH ₃ O	-3.5166
CH ₃ OH	-3.01366
CO ₂	-2.6055
COOH	-3.31943

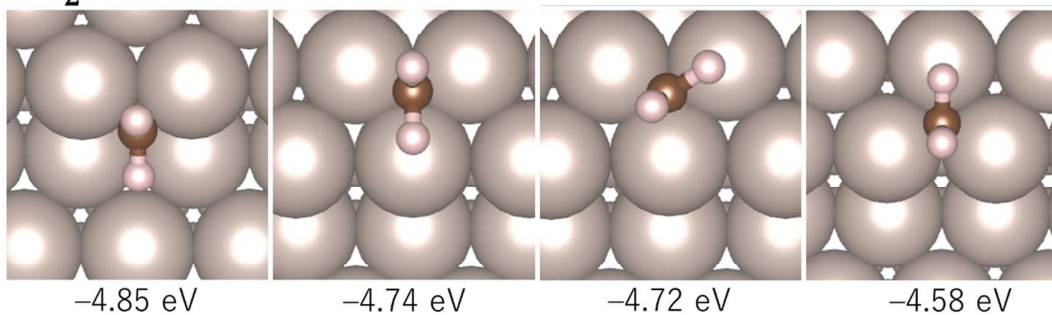
Figure S1 shows some other stable adsorption configurations of molecules with the corresponding adsorption energies.



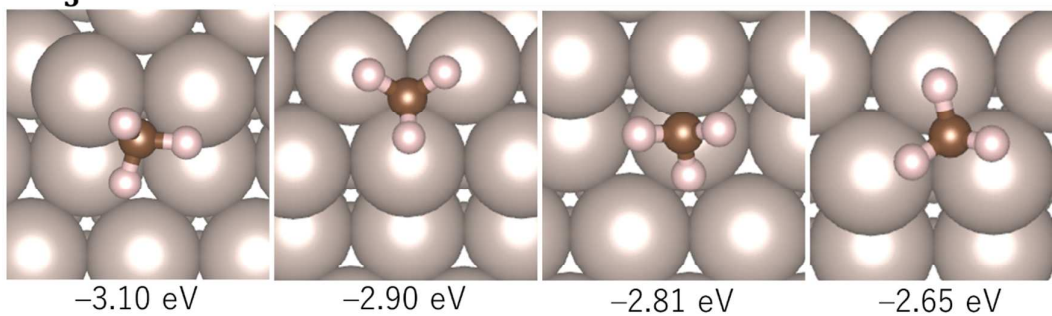
CH*



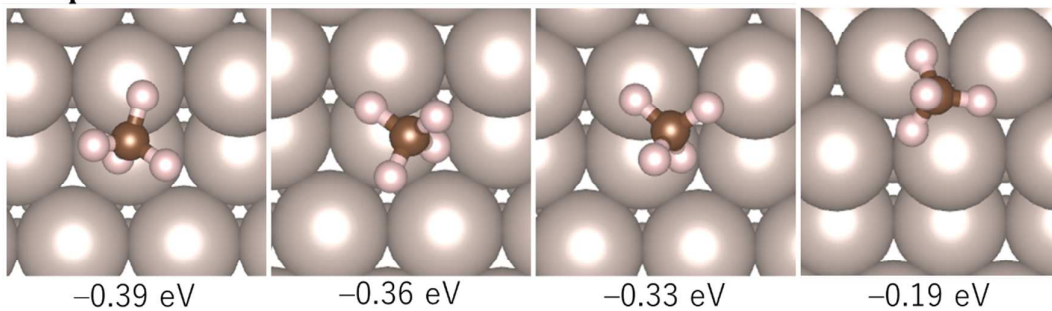
CH₂*



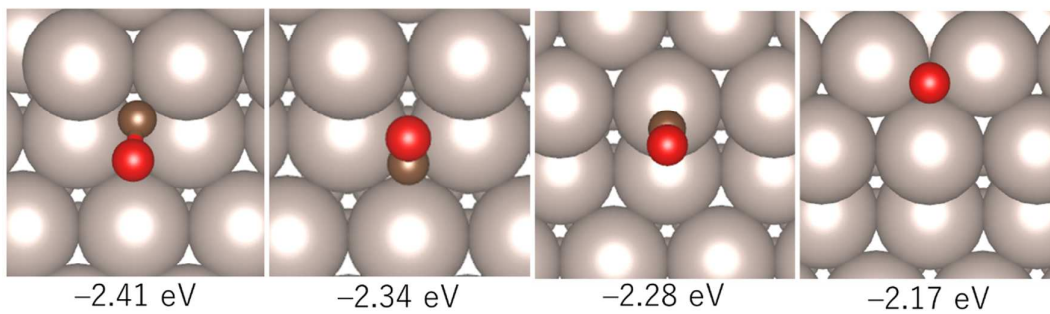
CH₃*



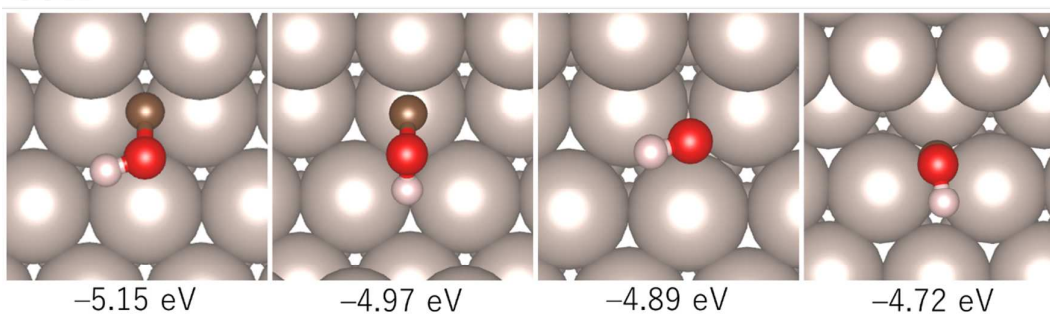
CH₄*



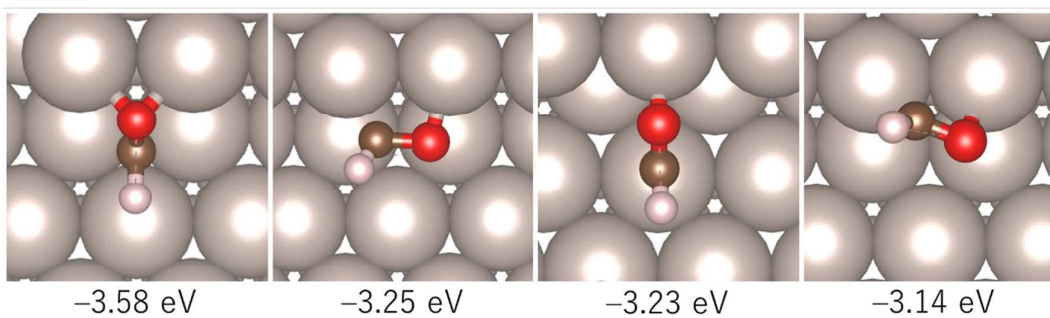
CO*



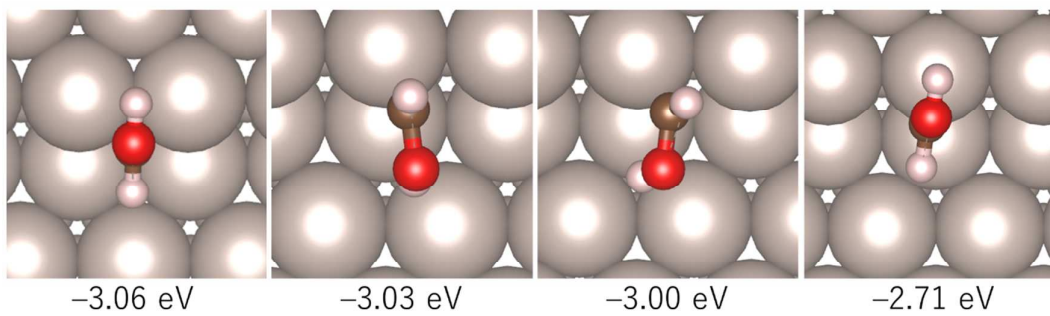
COH*



CHO*



CHOH*



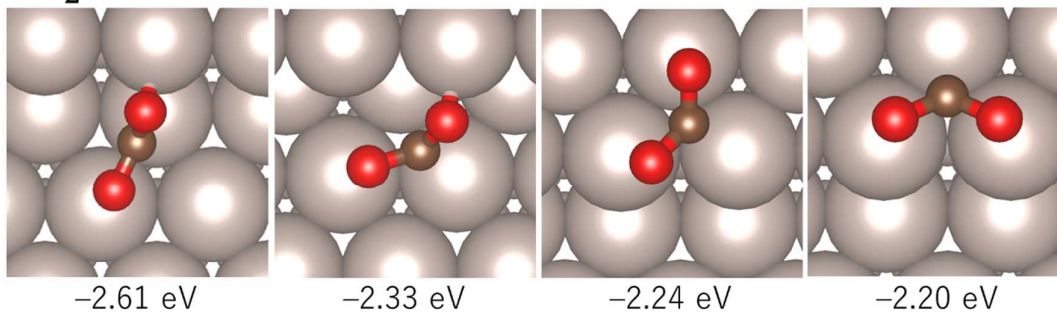
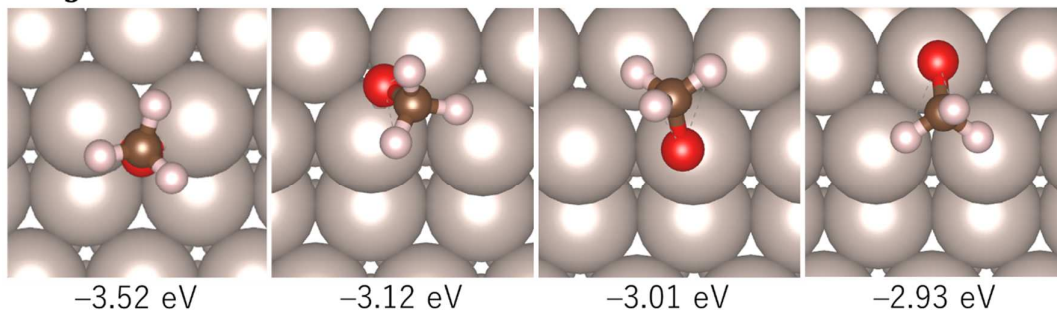


Figure S1: Other stable adsorption configurations of molecules and their adsorption energies.