

Fig. S1. The configuration of CH₃OH and corresponding intermediates involved in the CH₃OH cracking reaction on the Cu@C₂₄B₈ surface are shown. Gray, pink, red, and white respectively represent carbon atoms, boron atoms, oxygen atoms, and hydrogen atoms, with Cu atom inside.

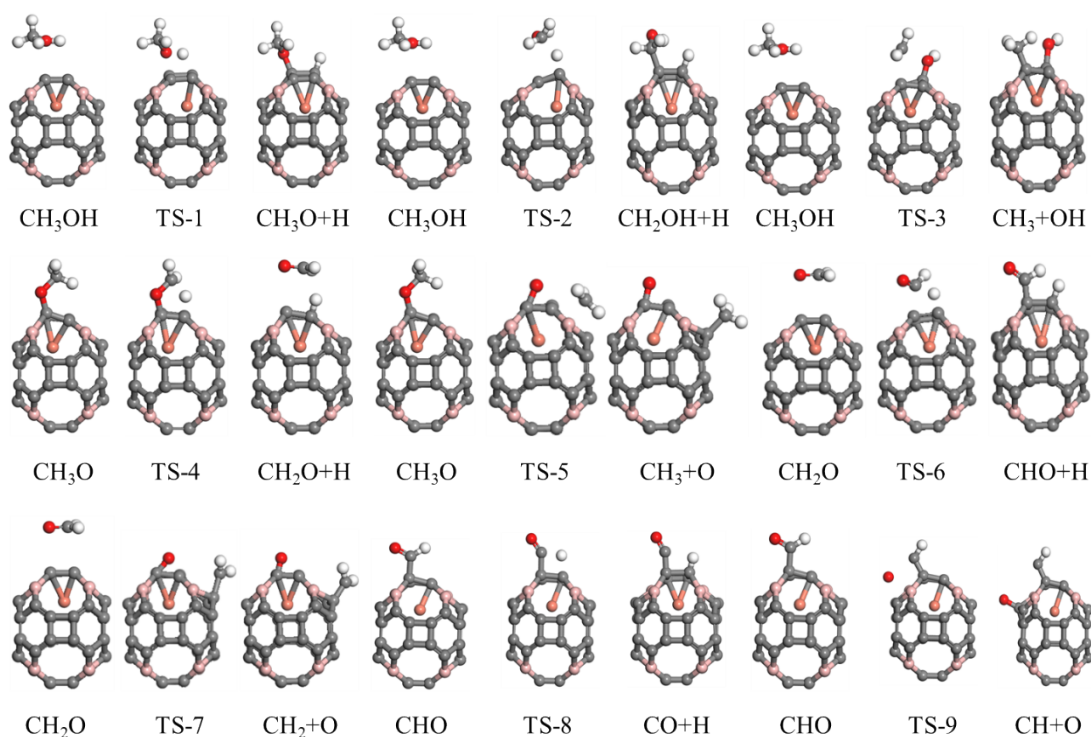


Fig. S2. The configuration of CH₃OH and corresponding intermediates involved in the CH₃OH cracking reaction on the Cu@C₄₀B₈ surface are shown. Gray, pink, red, and white respectively represent carbon atoms, boron atoms, oxygen atoms, and hydrogen atoms, with Cu atom inside.

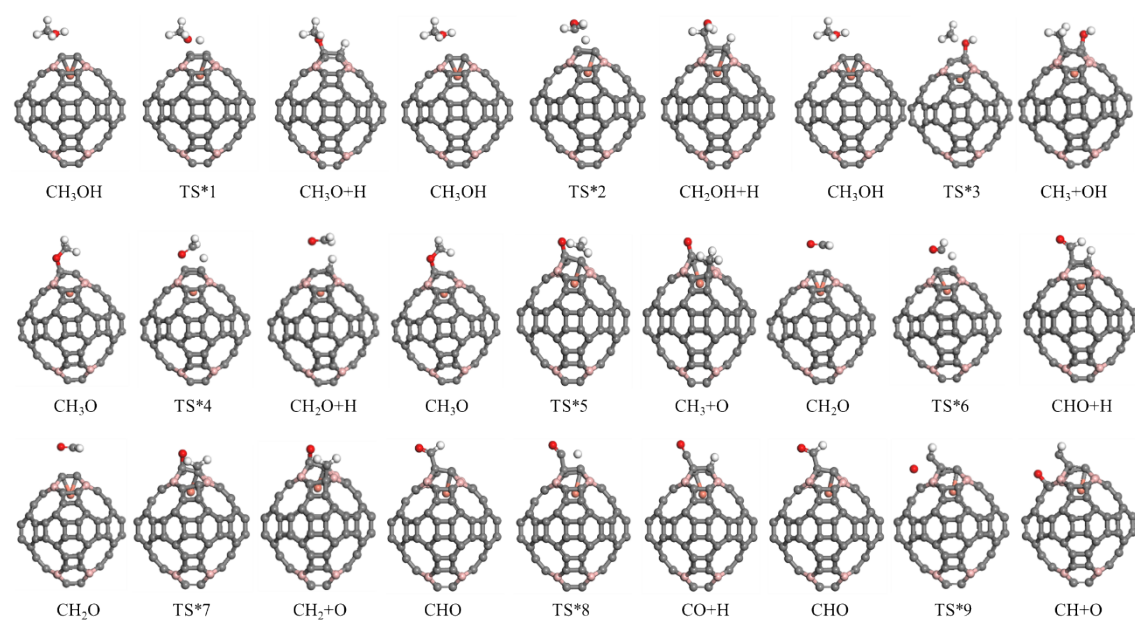


Fig. S3. The configuration of CH₃OH and corresponding intermediates involved in the CH₃OH cracking reaction on the Cu@C₈₈B₈ surface are shown. Gray, pink, red, and white respectively represent carbon atoms, boron atoms, oxygen atoms, and hydrogen atoms, with Cu atom inside.