

Supporting Information

For

Periodic DFT Study of the Donor Interactions with the MgCl₂ Surface in the Ziegler-Natta Catalytic System

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1. The figures of the optimized structures.

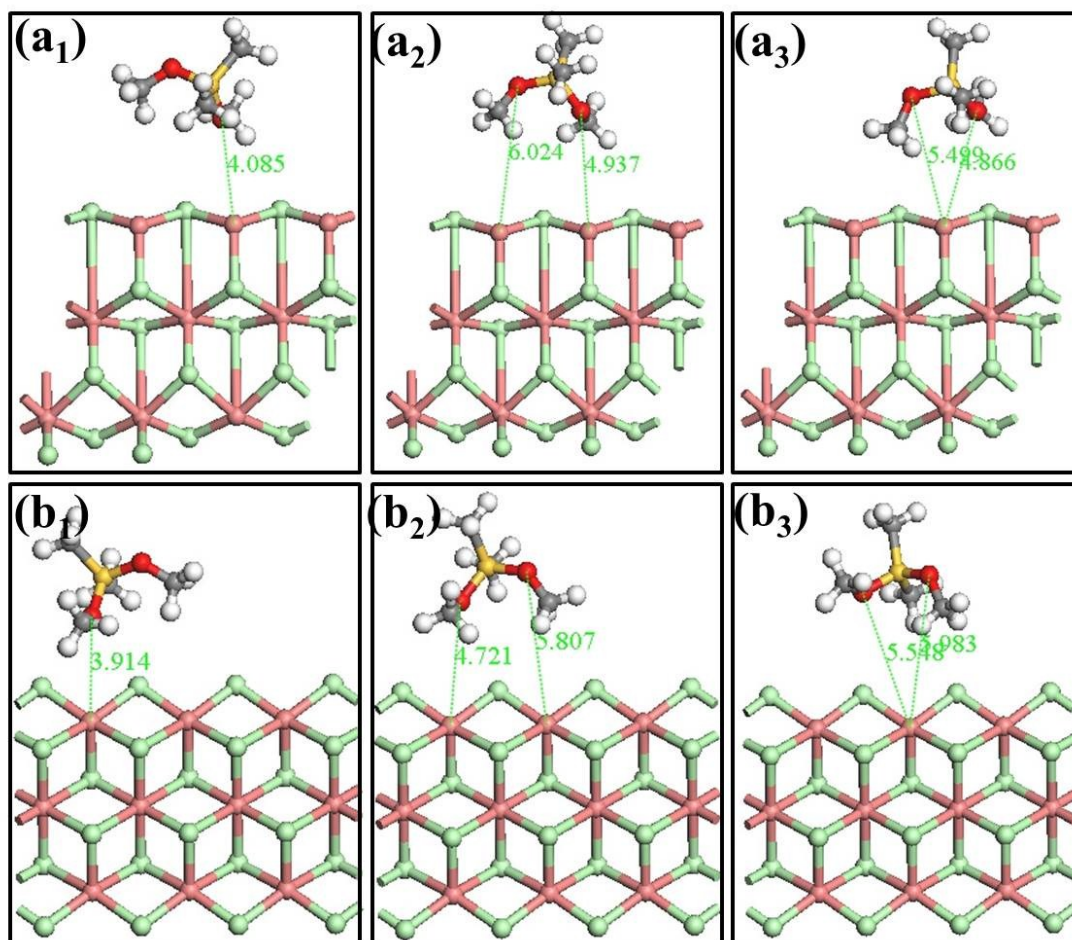


Fig. S1 Optimized structures of DMDS/ α -MgCl₂ (100) complexes, a_{1~3} is tri-coordinate, b_{1~3} is five-coordinate.

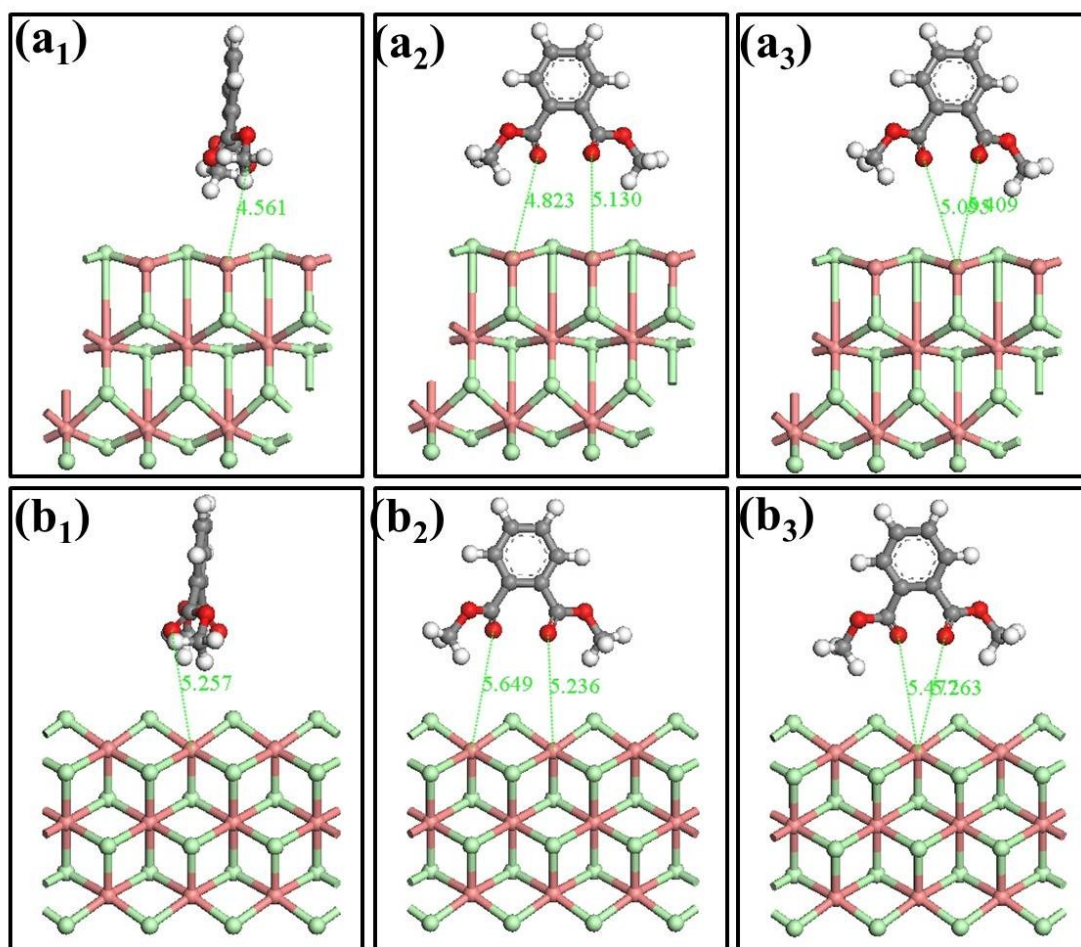


Fig. S2 Optimized structures of DMP/ α -MgCl₂ (100) complexes, a_{1~3} is tri-coordinate, b_{1~3} is five-coordinate.

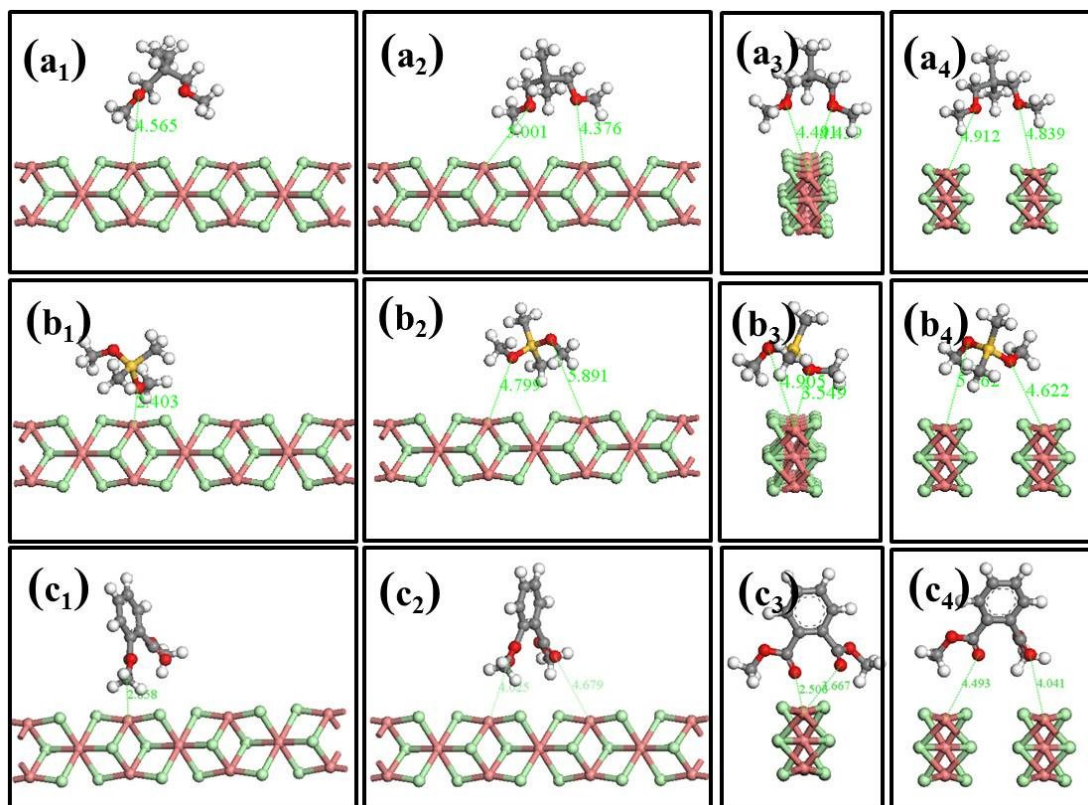


Fig. S3 Optimized structures of DMDP/ β -MgCl₂ (110), DMDS/ β -MgCl₂ (110), and DMP/ β -MgCl₂ (110) complexes: Mono-coordination (a₁, b₁, c₁), bridge coordination (a₂, b₂, c₂), chelate coordination (a₃, b₃, c₃), and zip coordination (a₄, b₄, c₄) modes.

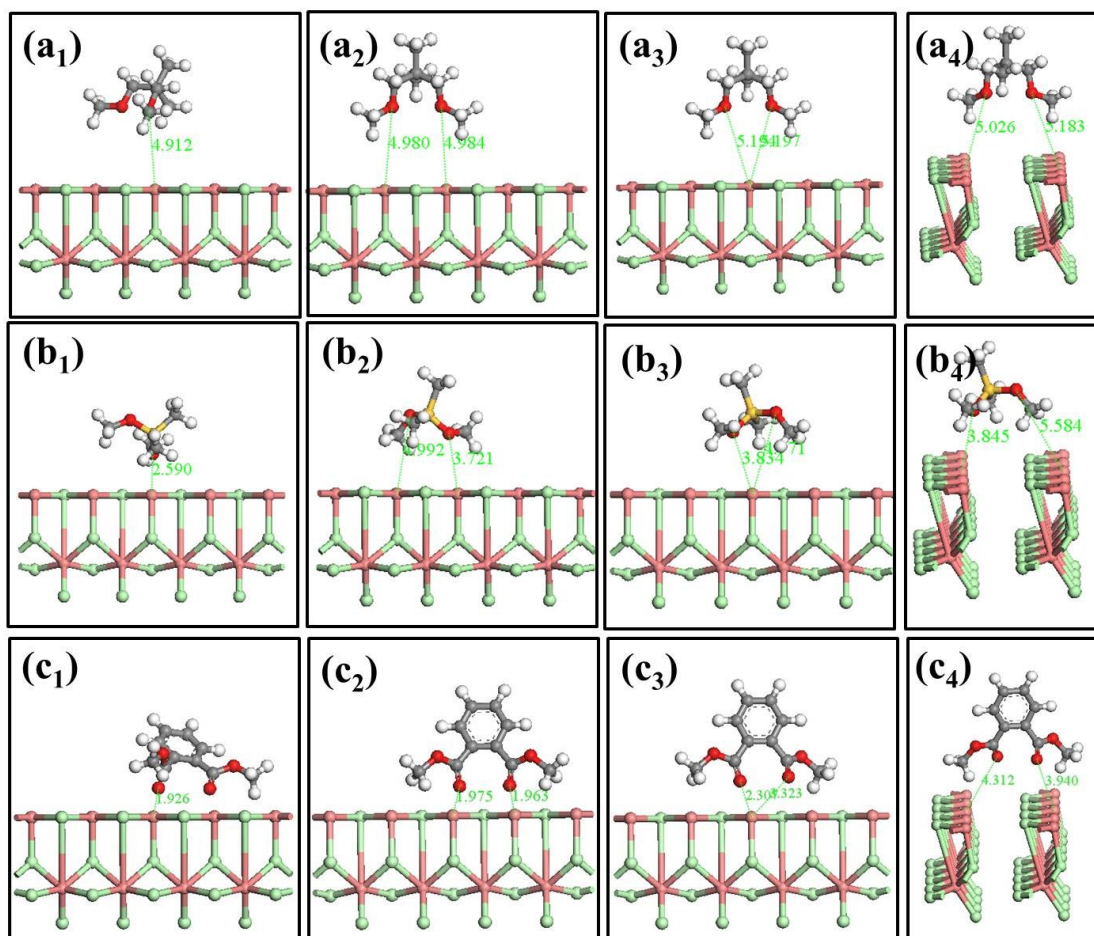


Fig. S4 Optimized structures of DMDP/ β -MgCl₂ (100) (a₁~₄), DMDS/ β -MgCl₂ (100) (b₁~₄) and DMP/ β -MgCl₂ (100) (c₁~₄) complexes.