

Supplementary Information

Double metal synergistic synthetic urea: A Electrocatalytic Study

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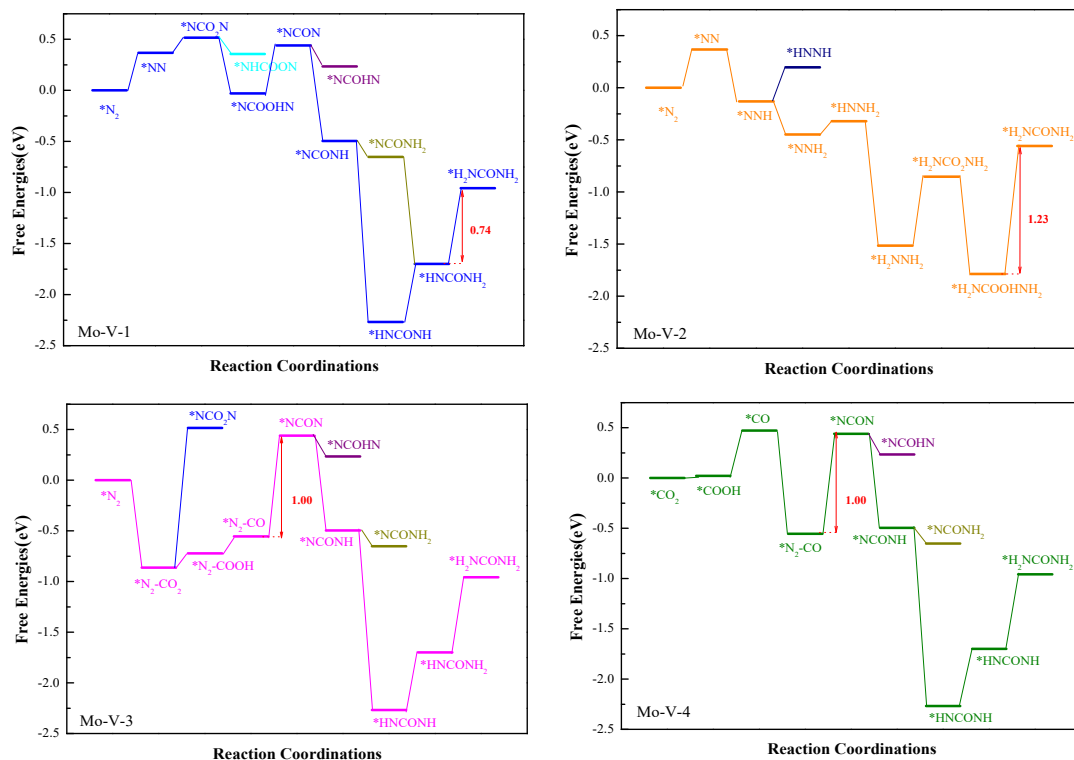


Figure S1 Different paths of urea synthesis on MoVN₆C, and the rate-limiting steps of each path are marked with red numbers.

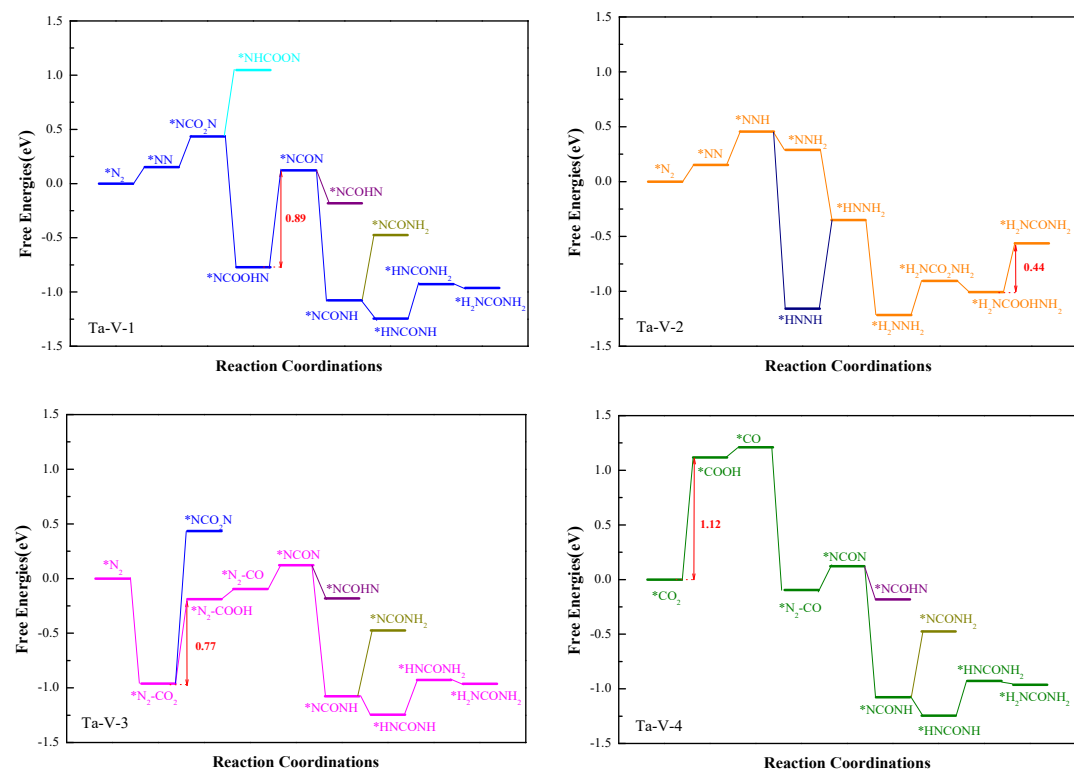


Figure S2 Different paths of urea synthesis on TaVN₆C, and the rate-limiting steps of each path are marked with red numbers.

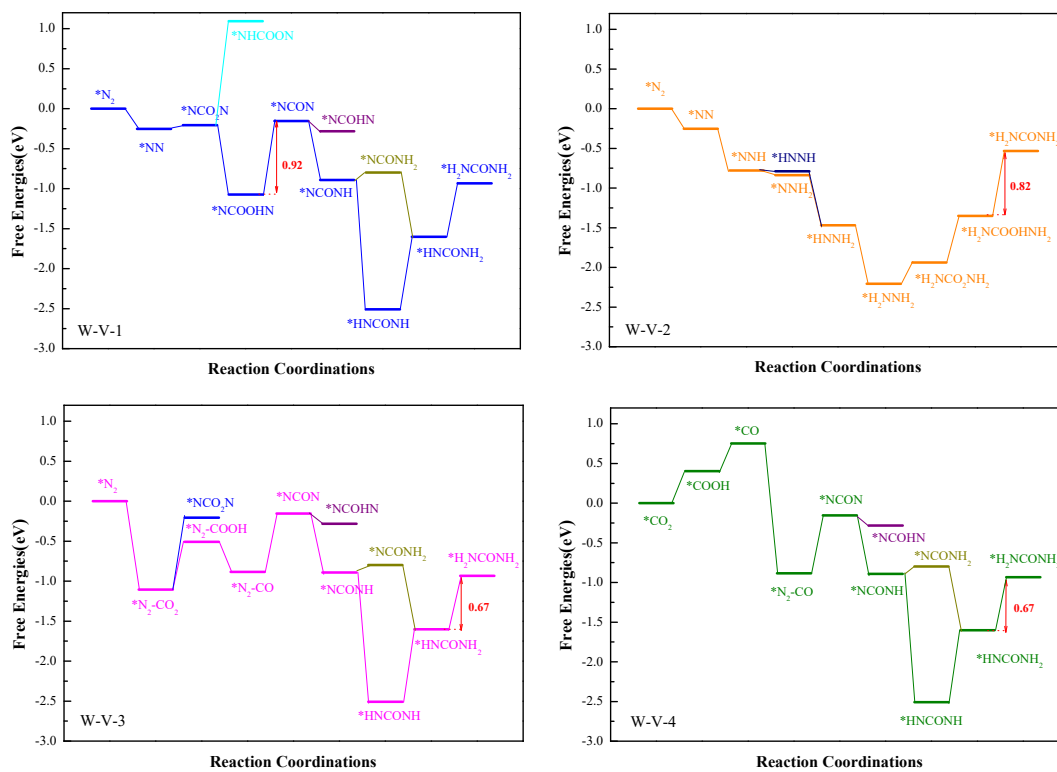


Figure S3 Different paths of urea synthesis on WVN₆C, and the rate-limiting steps of each path are marked with red numbers.

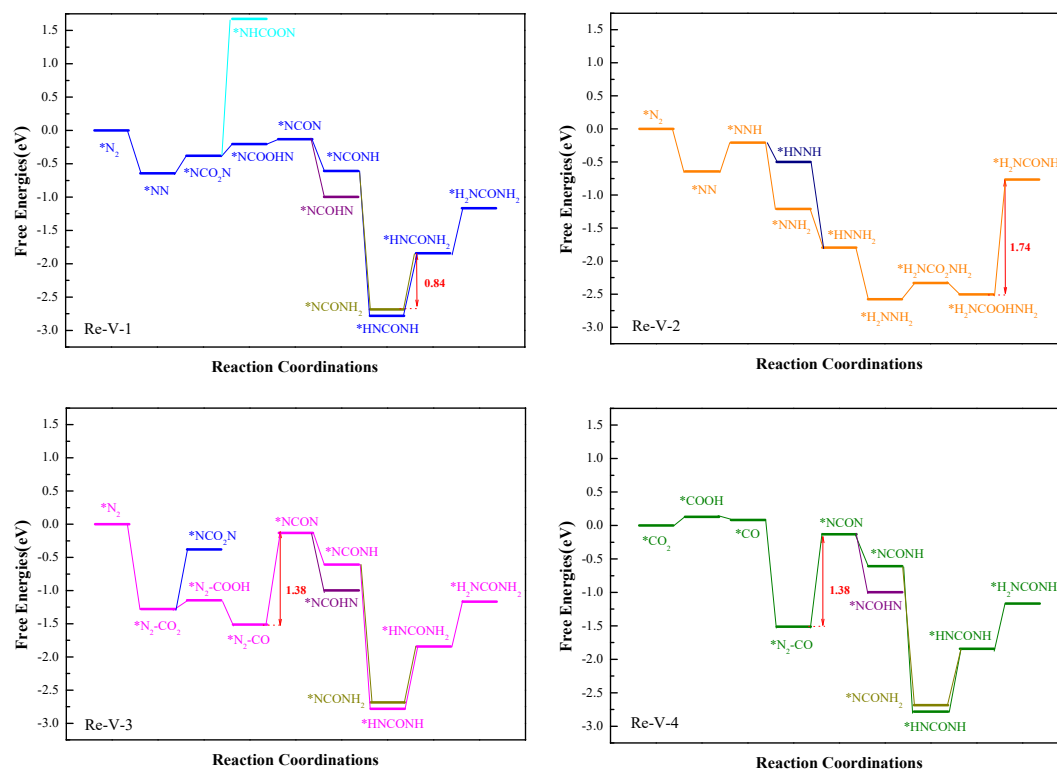


Figure S4 Different paths of urea synthesis on ReVN₆C, and the rate-limiting steps of each path are marked with red numbers.

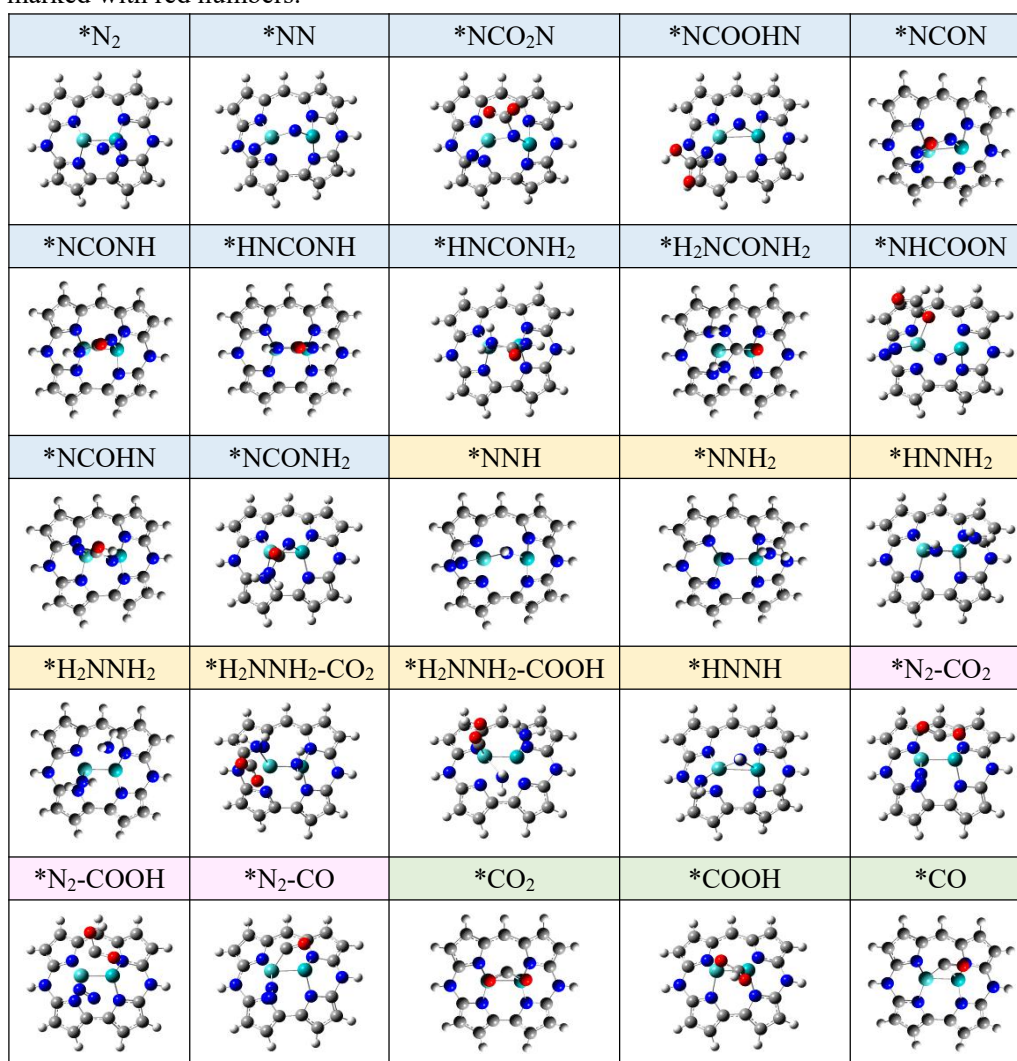
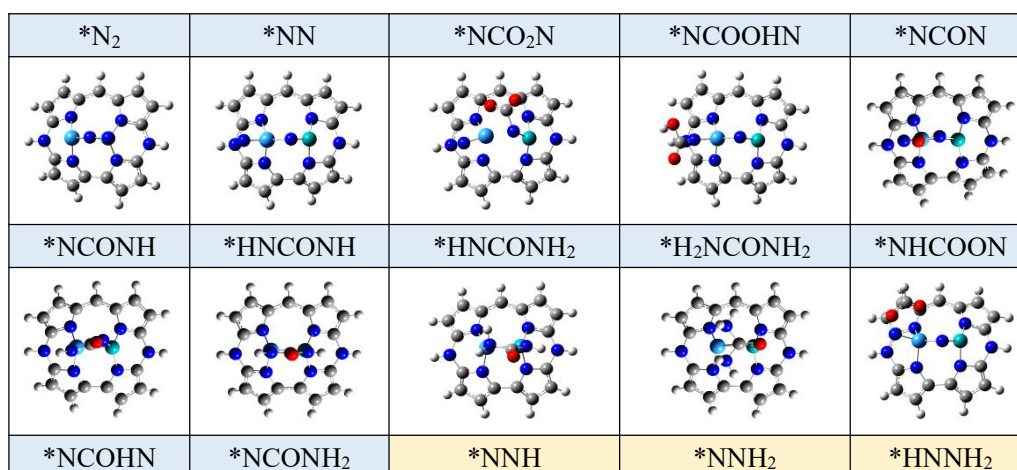


Table S1 There are 25 geometric structures corresponding to different paths of urea synthesis on MoVN₆C. Different shading colors (blue, orange, pink, green) represent four different paths.




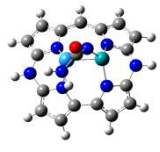

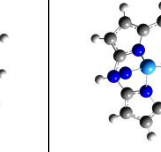
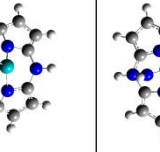

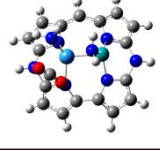
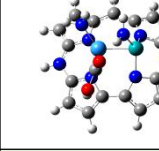
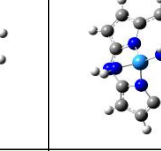
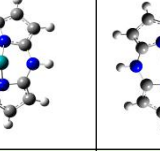
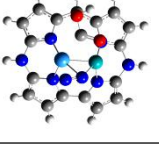
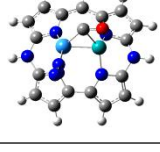
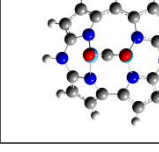
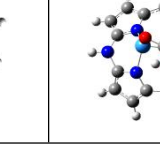
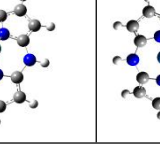



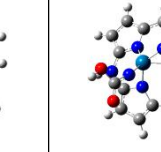
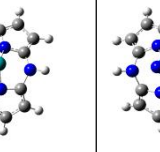
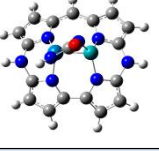

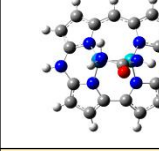
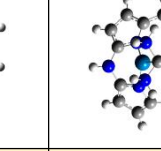
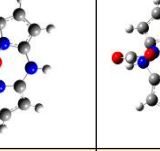
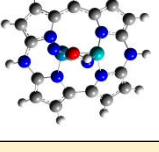
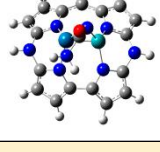
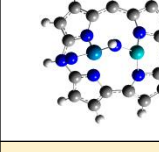
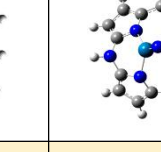
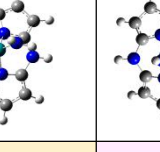
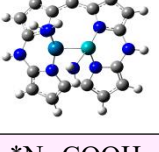
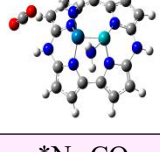
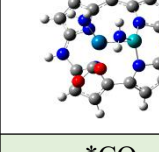
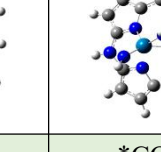
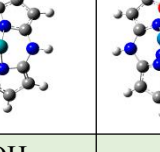
				
*H ₂ NNH ₂	*H ₂ NNH ₂ -CO ₂	*H ₂ NNH ₂ -COOH	*HNNH	*N ₂ -CO ₂
				
*N ₂ -COOH	*N ₂ -CO	*CO ₂	*COOH	*CO
				

Table S2 There are 25 geometric structures corresponding to different paths of urea synthesis on TaVN₆C. Different shading colors (blue, orange, pink, green) represent four different paths.

*N ₂	*NN	*NCO ₂ N	*NCOOHN	*NCON
				
*NCONH	*HNCONH	*HNCONH ₂	*H ₂ NCONH ₂	*NHCOON
				
*NCOHN	*NCONH ₂	*NNH	*NNH ₂	*HNNH ₂
				
*H ₂ NNH ₂	*H ₂ NNH ₂ -CO ₂	*H ₂ NNH ₂ -COOH	*HNNH	*N ₂ -CO ₂
				
*N ₂ -COOH	*N ₂ -CO	*CO ₂	*COOH	*CO

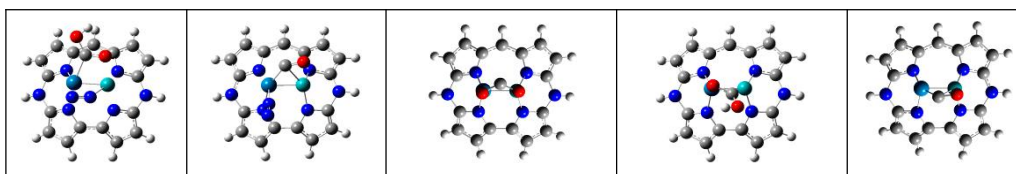


Table S3 There are 25 geometric structures corresponding to different paths of urea synthesis on WVN₆C. Different shading colors (blue, orange, pink, green) represent four different paths.

*N ₂	*NN	*NCO ₂ N	*NCOOHN	*NCON
*NCONH	*HNCONH	*HNCONH ₂	*H ₂ NCONH ₂	*NHCOON
*NCOHN	*NCONH ₂	*NNH	*NNH ₂	*HNNH ₂
*H ₂ NNH ₂	*H ₂ NNH ₂ -CO ₂	*H ₂ NNH ₂ -COOH	*HNNH	*N ₂ -CO ₂
*N ₂ -COOH	*N ₂ -CO	*CO ₂	*COOH	*CO

Table S4 There are 25 geometric structures corresponding to different paths of urea synthesis on ReVN₆C. Different shading colors (blue, orange, pink, green) represent four different paths.