Electronic Supplementary Information

Structural dynamics of Ru cluster during nitrogen dissociation in ammonia synthesis

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Contents

Fig. S1 Kinetic energy partitioning.....S3

Fig. S2 Probability distributions and mean forces obtained by different sampling methods.....S4

Fig. S3 PMF curves at different temperatures.....S5

Fig. S4 Average forces at different N-N bond lengths S6

Fig. S5 Hysteresis of mean force.....S7

Fig. S6 Specific heat capacity curves.....S8

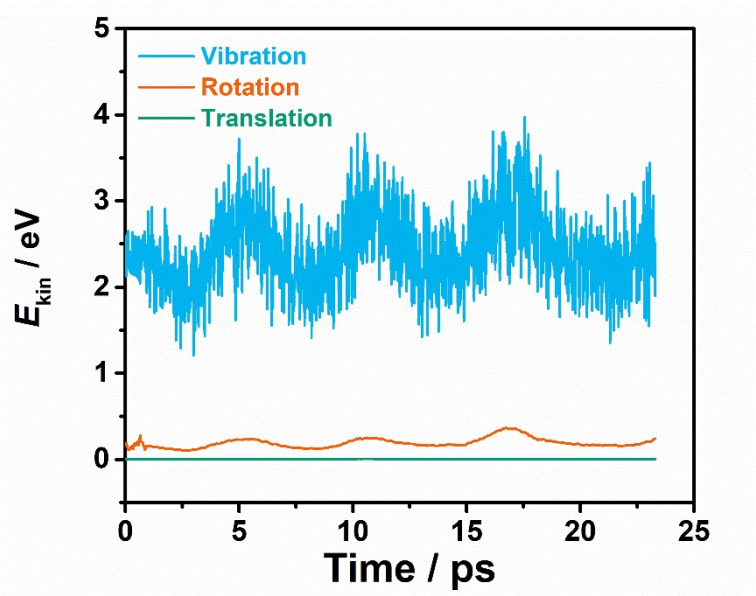

Fig. S1. Kinetic energy partitioning for the Ru-N_2 system thermostated by Nosé–Hoover chain at 523 K. The N-N bond length is controlled to 1.84 Å.

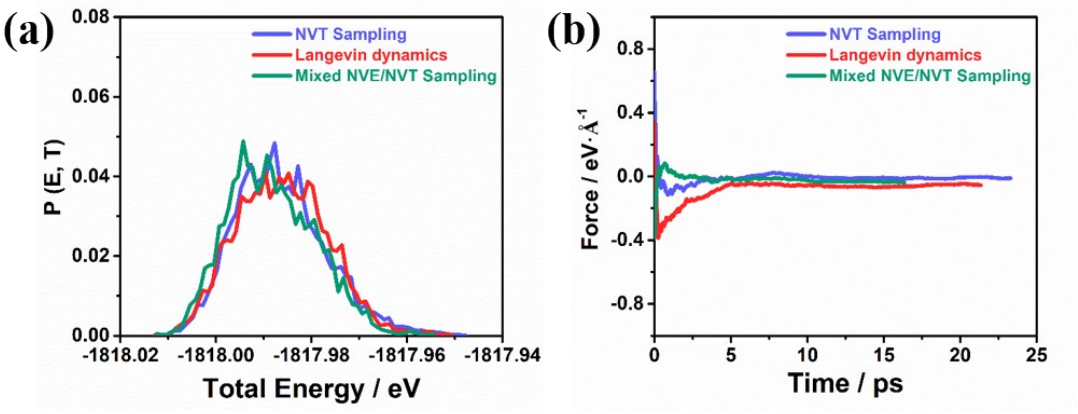

Fig. S2. (a) Total energy probability distributions P (E, T) and (b) the time accumulative averages of mean forces obtained by NVT combined with Nosé−Hoover chain thermostat with a chain length of three (blue line), the Langevin dynamics (red line), and mixed NVE/NVT sampling (green line) at 523 K. The N-N bond length is controlled to 1.84 Å. The probability distributions and mean forces between NVT and mixed NVE/NVT sampling are very similar, indicating that the interference issue due to the coupling the internal degrees of freedom of the cluster with a thermostat in this work is insignificant.

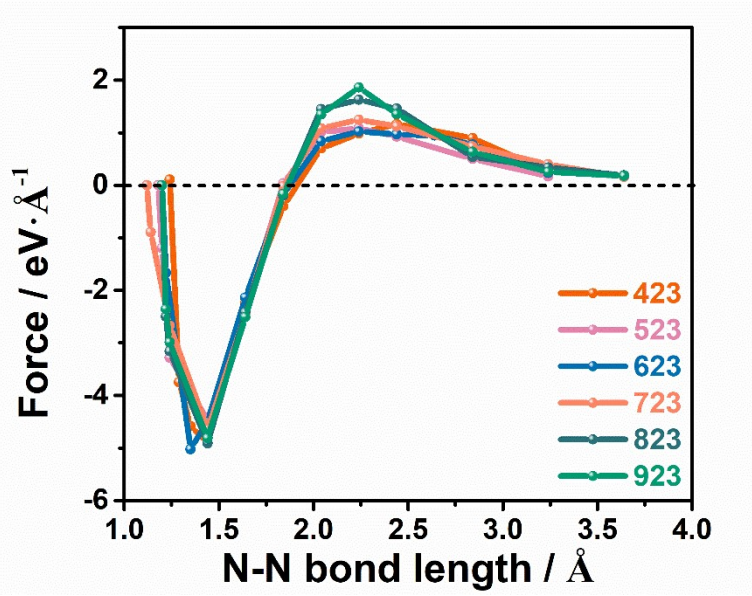

Fig. S3. Calculated average forces for N_2 dissociation on Ru_{19} cluster as a function of N-N bond length at different temperatures (unit: K).

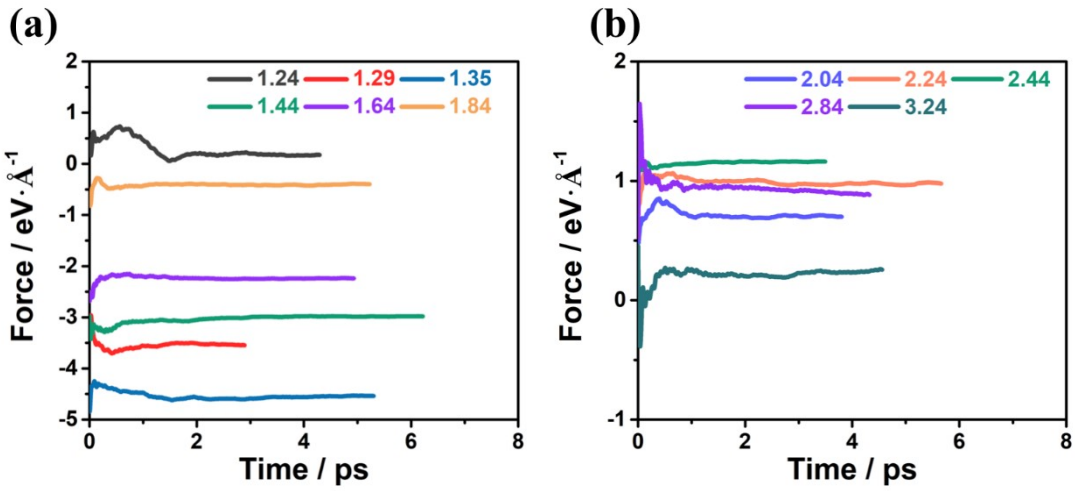

Fig. S4. (a) Time accumulative averages of the forces at the N-N bond length varying from 1.24 Å to 1.84 Å and (b) from 2.04 Å to 3.24 Å at 423 K calculated using AIMD. The inset values are the corresponding N-N bond lengths given in Å.

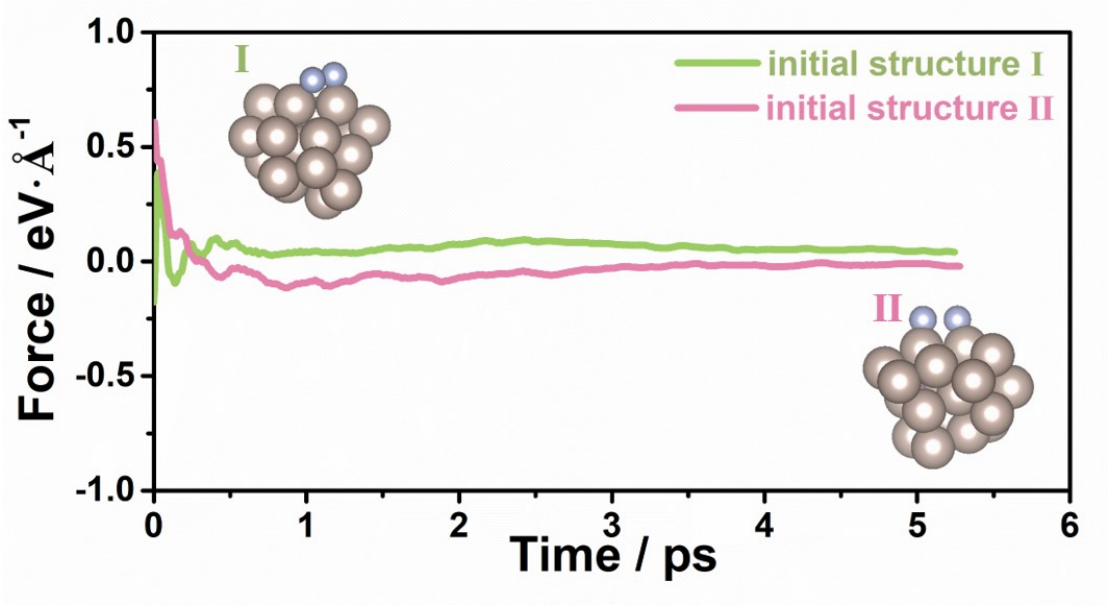

Fig. S5. Time accumulative averages of mean forces at the N-N bond length of 1.84 Å calculated using different initial structures at 523 K. The inserts are the snapshots of initial structures. I, the N-N bond length is 1.44 Å. II, the N-N bond length is 2.04 Å. The silver and blue balls represent Ru and N atoms.

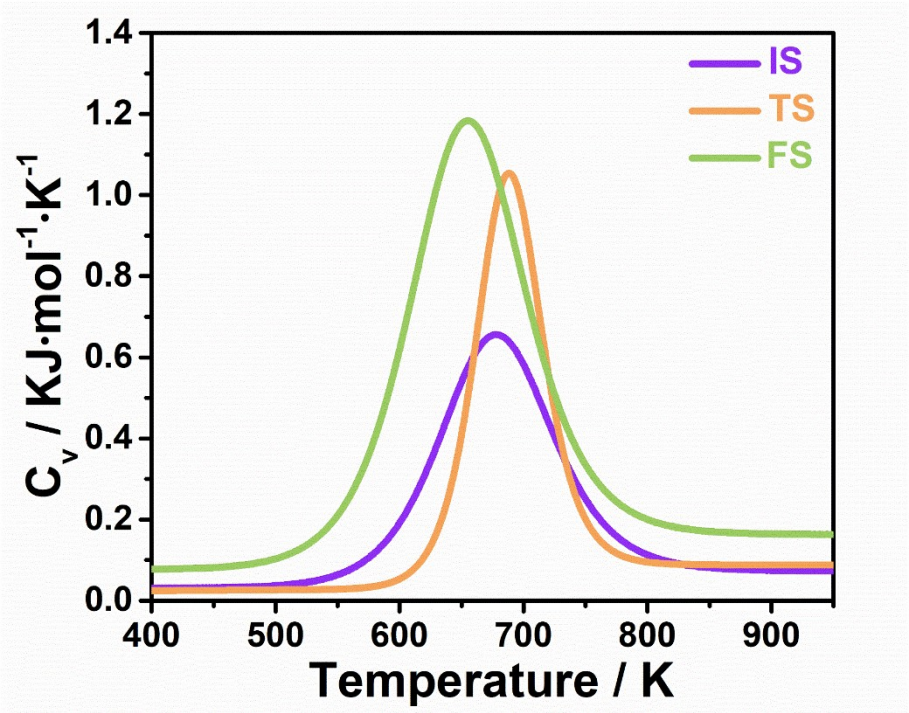

Fig. S6. Specific heat capacity curves of initial (IS), transition (TS), and finals states (FS) of the N_2 dissociation on Ru_{19} cluster.