

CBe₄H₆: A molecular rotor with a built-in on-off Switch

Bo Jin,^{abc} Caixia Yuan,^{ab} Jin-Chang Guo,^{ab} and Yan-Bo Wu^{*ab}

^a *Key Laboratory of Materials for Energy Conversion and Storage of Shanxi Province, Institute of Molecular Science, Shanxi University, 92 Wucheng Road, Taiyuan, Shanxi, 030006, People's Republic of China.*

^b *Key Laboratory of Chemical Biology and Molecular Engineering of Ministry of Education, Institute of Molecular Science, Shanxi University, 92 Wucheng Road, Taiyuan, Shanxi, 030006, People's Republic of China.*

^c *Department of Chemistry, Xinzhou Normal University, 1 East Dunqi Street, Xinzhou, Shanxi, 034000, People's Republic of China.*

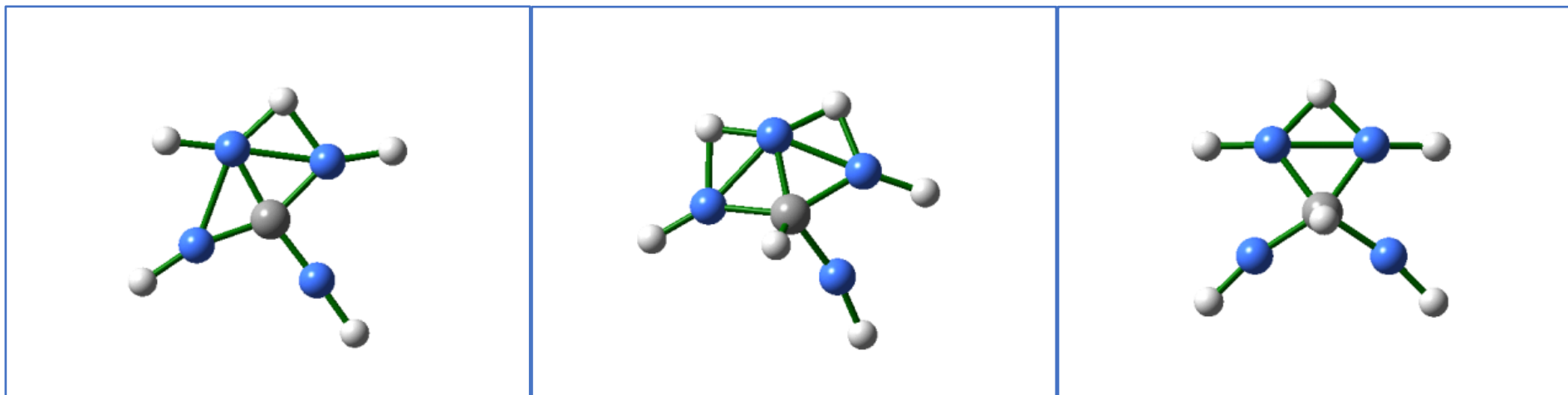
*To whom correspondence should be addressed.

mail: wyb@sxu.edu.cn (Y.B.W.)

SI-2 Videos for concerned vibrational modes, idealized rotational models, and trajectories of molecular dynamics simulations

Note: Please press [F5] to show the videos in the following slides.

Vibrational modes for lowest imaginary frequencies of transition states **TS1** and **TS2** as well as the second-order saddle point **2ndSP**

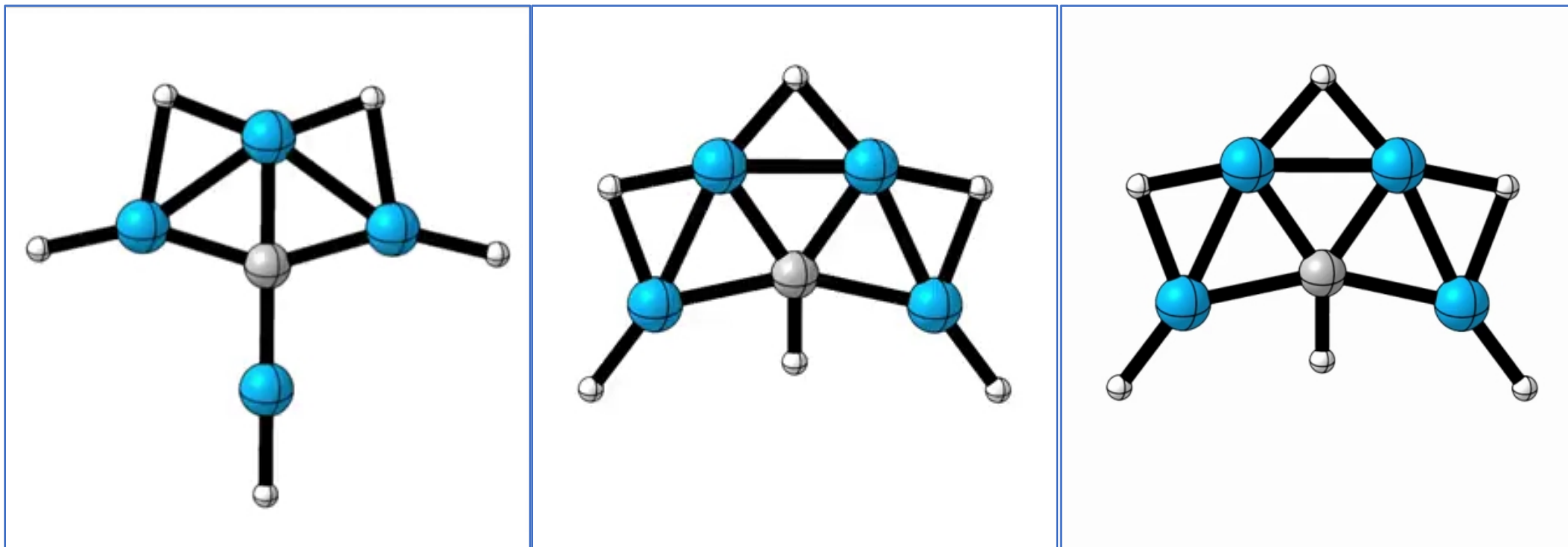


TS1

TS2

2ndSP

Idealized rotational model (the one-way rotations) of **1A**, **2A** and **working rotor model of 2A**



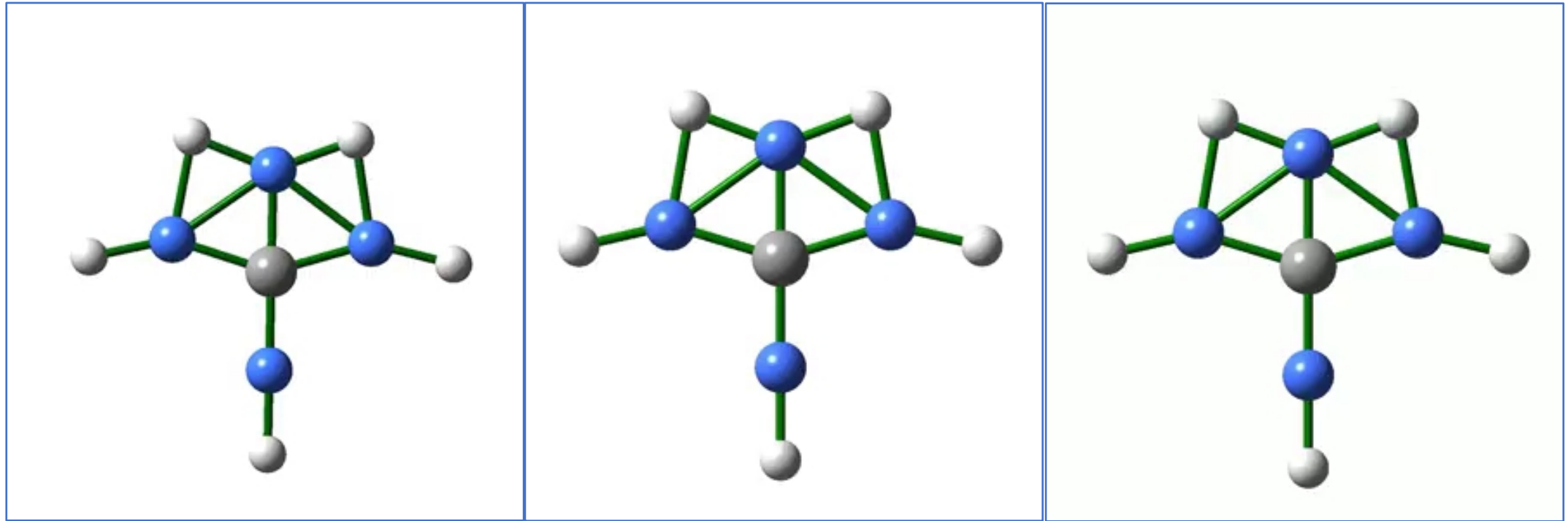
1A

2A

Working rotor model of 2A

Note: click the picture to view corresponding video if it does not automatically start

Selected structural evolution in BOMD trajectories of **1A**



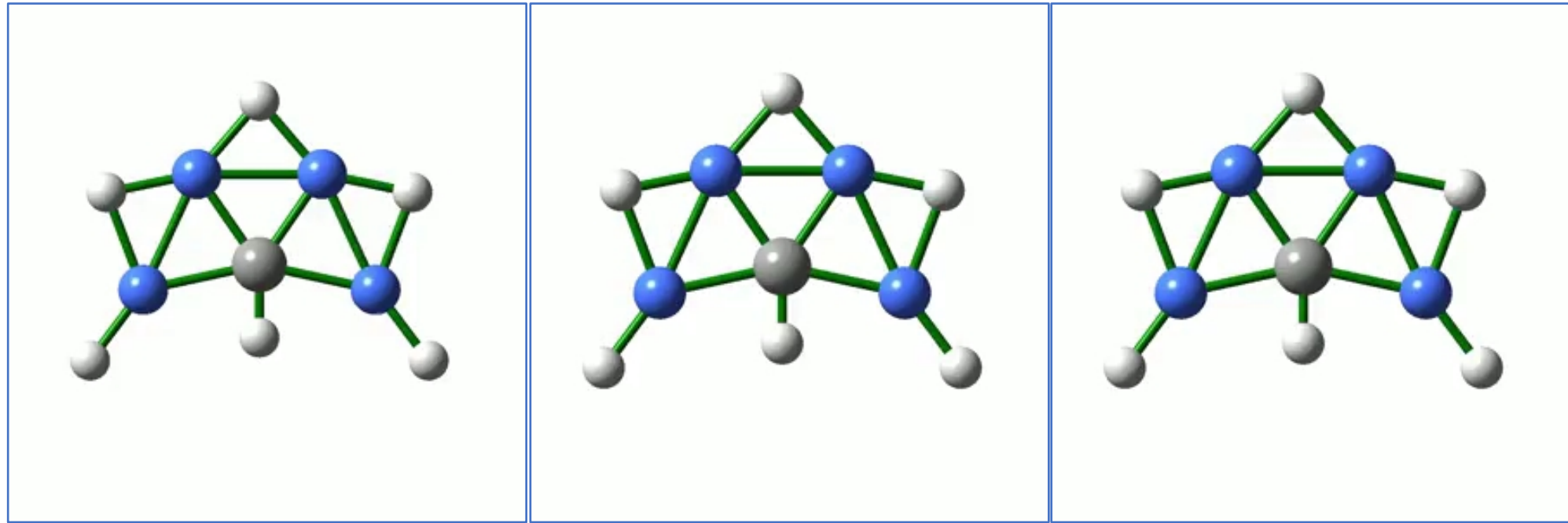
298 K

600 K

1000 K

Note: click the picture to view corresponding video if it does not automatically start

Selected structural evolution in BOMD trajectories of **2A**



298 K

600 K

1000 K

Note: click the picture to view corresponding video if it does not automatically start