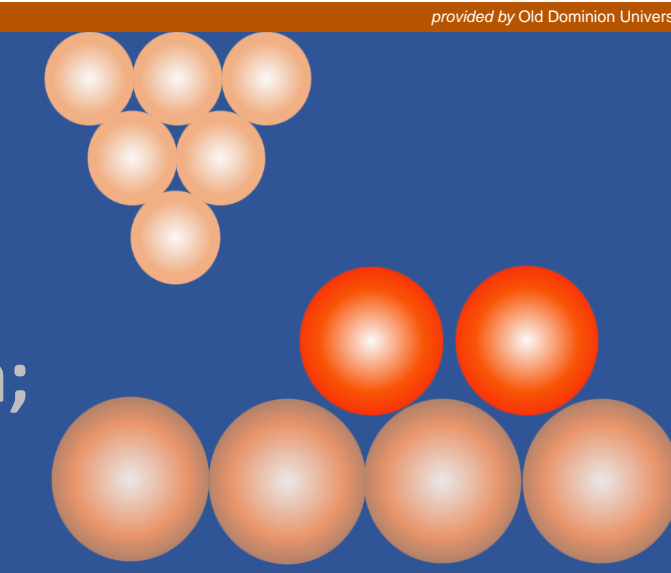


# Direct Visualization of 3-Dimensional Force and Energy Map of a Single Molecular Switch



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## ABSTRACT

Fundamental researches on mechanical and flexure properties of molecules adsorbed on materials surface can greatly advance applications of molecular thin films on devices. Here, we mechanically induce conformational change on a single molecule and quantify the driving force required for such molecular shape switch via a low temperature ( $\sim 5\text{K}$ ) Scanning Tunneling Microscope (STM) and Qplus Atomic Force Microscope (Q+AFM). Our measurement maps a three-dimensional landscape for mechanical potential and force at single molecule level with high spatial resolution of a few angstrom ( $10^{-10}\text{m}$ ) in all three dimensions. Our preliminary results indicate that an energy barrier of  $\sim 400\text{meV}$  needs to be overcome for rings flipping of TBrPP-Co.

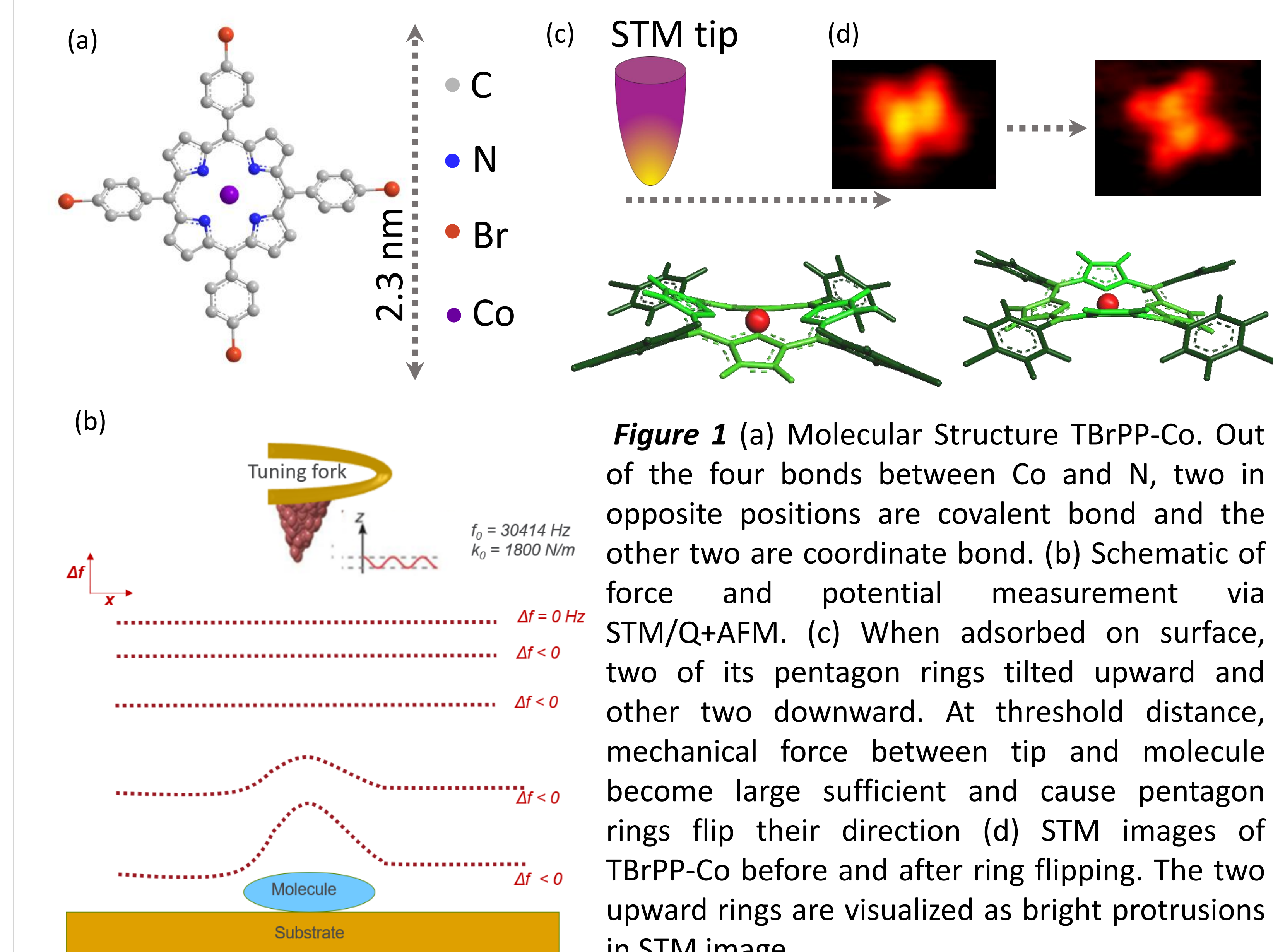
## METHODOLOGY

### Sample Preparation

- A single crystal metal substrate Au(111) is cleaned to atomic level by repeated cycles of  $\text{Ar}^+$  ion bombardment and annealing at  $\sim 600^\circ\text{C}$ .
- Molecule TBrPP-Co is subsequently deposited on substrate via thermal evaporation in an ultra-high vacuum preparation chamber ( $\sim 10^{-9}\text{torr}$ ).

### Data Collection

- The fabricated sample is transferred to analysis chamber in-situ for manipulation experiment.
- A sharp Pt/Ir tip (apex radius of a few nanometers) is mounted on a fine tuning fork ( $\sim 1\text{mm}$  in length) and is driven to vibrate at  $f_0 = 30414\text{Hz}$ .
- Tip scans the molecule at different heights with  $0.1\text{\AA}$  as increment till approaches threshold distance, and meanwhile tip-molecule interaction strength is recorded in the form of tip frequency change  $\Delta f$ , a method first demonstrated by Ternes et al.<sup>1</sup>.
- At threshold distance, mechanical force between tip and molecule become large sufficient and cause pentagon rings flip their direction.
- Frequency change  $\Delta f$  is translated into vertical stiffness of the tuning fork, vertical force between tip and molecule, and potential energy of the molecule using Sader-Jarvis method<sup>2</sup>.
- By mapping a mechanical potential landscape for a single molecule TBrPP-Co with spatial resolution of a few angstrom in all three dimensions, the energy barrier to be overcome and force required for such molecular conformation switch can be quantified with accuracy of a few tens meV and a few pico-Newton pN.

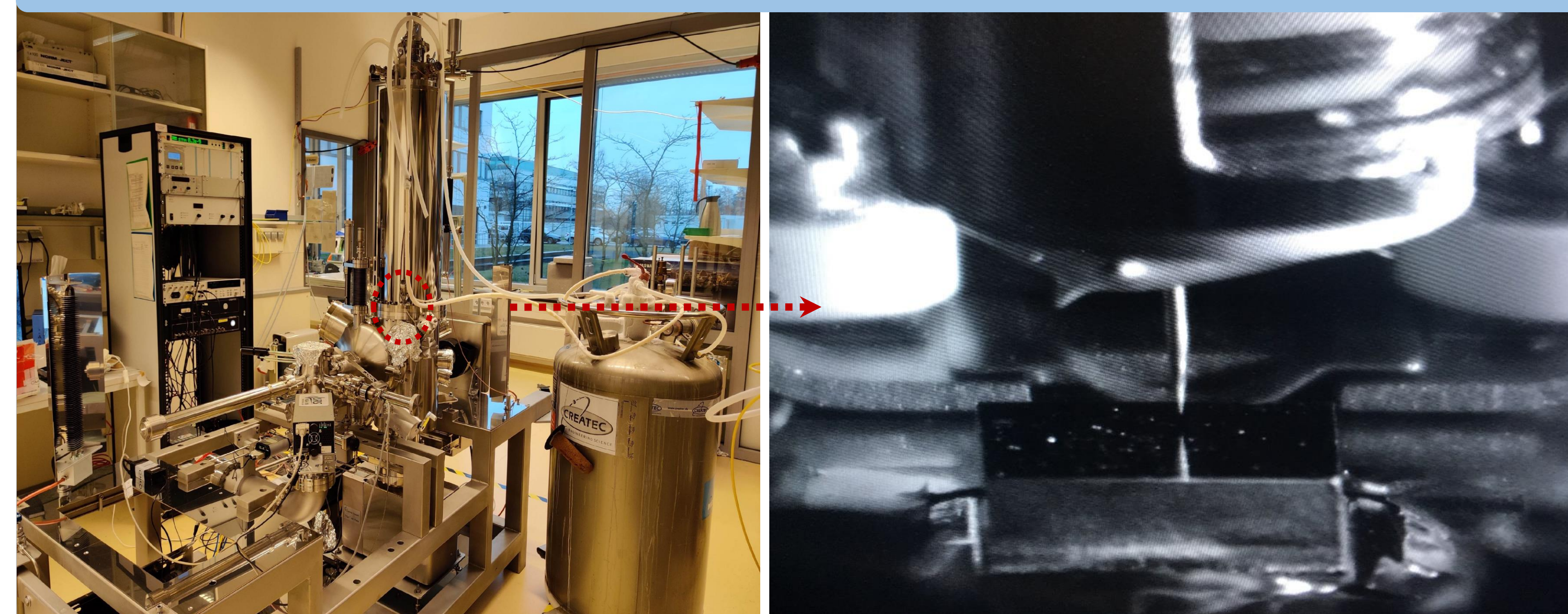


## ACKNOWLEDGEMENT

The STM experiments and analysis were supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, grant DE-FG02-02ER46012. A. M. S. D. W. is supported by Y. Z.'s start-up funding provided by ODU. Y.L. and K. Z. L. are supported by the US Department of Energy Office of Basic Energy Sciences (SISGR Grant DE-FG02-09ER16109). L.A.C. and A.T.N. were supported by the US Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering. We gratefully acknowledge the computer time from the Argonne National Laboratory Computing Resource Center (LCRC).

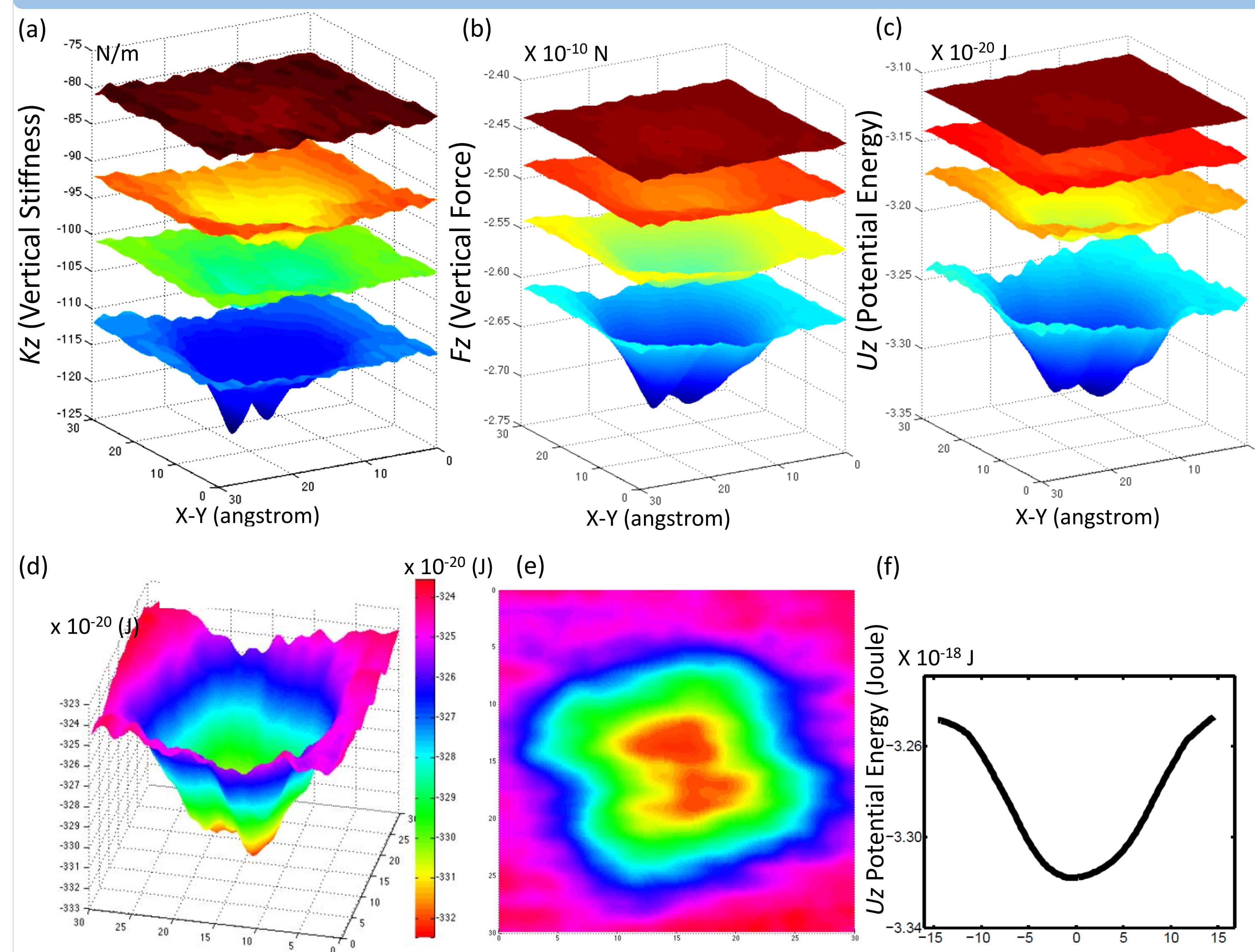
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## INSTRUMENT



**Figure 2** Left: Low Temperature Scanning Tunneling Microscope (STM) and Qplus Atomic Force Microscope (Q+AFM). Ultra-high vacuum:  $10^{-10}\text{torr}$ ; Temperature:  $4\text{K}$ . Red oval represents the area where scanning head is housed. Right: Scanning head of STM. Lateral spatial resolution of a few angstrom.

## EXPERIMENT RESULTS



## CONCLUSION & OUTLOOK

### Conclusion

- TBrPP-Co molecular conformation switch can be successfully induced in a mechanical manner via STM/Q+AFM.
- Our preliminary results indicate that an energy barrier of  $\sim 400\text{meV}$  needs to be overcome for rings flipping of TBrPP-Co.
- Results presented here are based on analysis of preliminary data. With more data collected and further analysis, results are subject to adjustment before research finalizing stage.

### Critical Questions Remain for Further Study

- Force direction for conformational switch needs to be identified. The study by Ternes et al.<sup>1</sup> reveals that lateral component  $F_x$  of the total force play the critical role in molecular movement across the surface. However, it is unclear if it is lateral  $F_x$  or vertical  $F_z$  component of the total force that cause molecular conformation change. Further analysis is needed.
- Theoretical calculations are ongoing to find whether conformational change is accompanied by bond change from covalent bond to coordinate bond.

## REFERENCE

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