

## **‘Spring-Like’ Molecular Junctions: An Avenue to Store Energy in Molecules to Power Molecular-Machines**

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### **ABSTRACT:**

Incorporation of the inherent molecular elasticity into molecular electronics (1-6) would enable development of next-generation molecular electromechanical systems like energy storage devices, molecular timers and actuators, which could be integrated to build self-sustaining molecular machines. However, the major challenges in achieving such molecular-mechanics are (a) applying confined and precise forces on the molecular-junction, (b) fabricating a molecular-junction with strong (multiple) bonds which can sustain mechanical deformation and (c) having a non-rigid system at molecular scale with sufficient mobility to achieve unrestrained mechanics. Such molecular mechanics cannot be achieved in a device construct where molecular junctions are incorporated between rigid electrodes.

As a part of this presentation, we will demonstrate (a) a working “molecular-spring” nanodevice, (b) a mechanism to controllably apply confined forces on molecular junctions, and (c) a molecular system which can store compression and stretching energy. Here, the molecular spring system is built with crosslinked polyallylamine-hydrochloride (cPAH) molecules sandwiched between 30 nm gold nanoparticles (GNP), where cPAH molecular-junctions are reversibly compressed and stretched by applying electrically and centrifugally induced forces respectively, while GNPs play a dual role (a) of movable connectors to apply forces and (b) of nanoelectrodes to measure molecular deformation via change in electron tunneling conductivity(7-9). The system functions like a ‘molecular-spring’, where the compression and stretching energy of the junctions can be stored and used to apply forces on the nanoparticles to bring them back to their native state. The dynamics of both externally and internally induced molecular motion fits well with the equation of spring in viscous media.

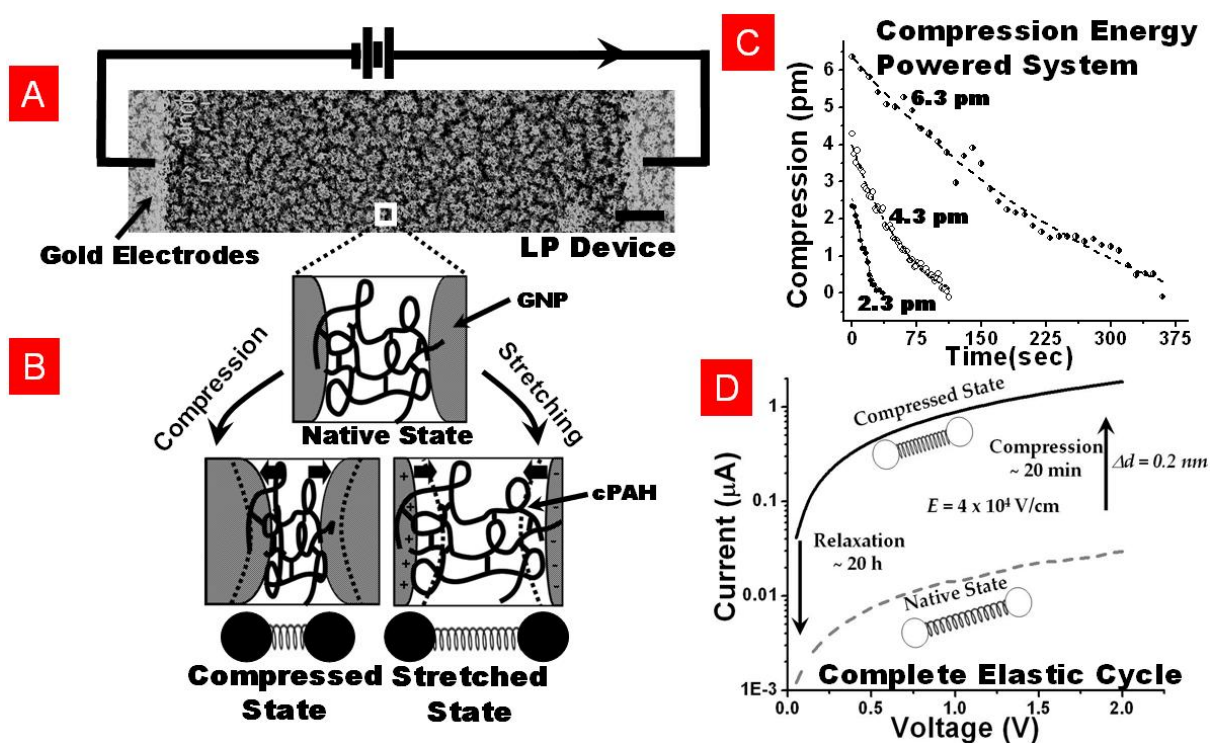
In the second part of the presentation, we will present a light-actuated molecular junction built by incorporating azo-group containing molecular junctions between metal-nanoparticles. Here, the mechanical actuation of azo-group is induced via exposure to light of wavelength 365 nm and 420 nm and is used to controllably manipulate the attached nanoparticles. The dynamics of reversible light-induced-actuation of nanoparticles (by ~0.2 nm) will also be demonstrated.

As an enabling technology, the outcome of these results will benefit a wide range of scientific disciplines and push the frontier of molecular-mechanics and nanotechnology. The ability to store compression energy in a molecular-device-architecture has the potential to power future molecular devices by stored molecular-energy. Further, the azo-group mechanics could be used to manipulate nanoparticles, thus controlling properties of nanocomponent based devices.

## Reference List

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## Figures:



**Figure A.** FESEM micrograph of a typical molecular-spring device between gold electrodes connected to a power supply. Scale bar = 100 nm. **B.** Schematic representation of compression and stretching of cPAH junctions between GNPs. **C.** Compressed molecules upon release of forces use the stored compression energy to push nanoparticles back to their native state with the rate of relaxation governed by the magnitude of the stored compression energy. Molecules compressed by ~2.3 pm, ~4.3 pm and ~6.3 pm, relaxes back to its original state in ~0.5 min, ~2 min and ~6 min respectively. **D.** Complete compression-relaxation cycle of a molecular spring device with the two conductivity states is shown.