

Electron Diffraction Imaging of Molecular Nanostructures and Molecular Motions

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Atomic resolution imaging of single molecules is a grand challenge in nanoscience where direct observation at Ångstrom resolution is the ultimate goal in nanostructure characterization. However, atomic resolution electron imaging is limited by the undesirable effects induced by electron beam irradiation. Thus, reducing the irradiation damage has been the driving force for the development of lower acceleration voltage, aberration corrected transmission electron microscopy (TEM) and scanning transmission electron microscopy. Here we will report progress made at University of Illinois on electron diffraction and imaging of molecular nanostructures using C₆₀ molecules confined in single wall carbon nanotubes (peapods) as model system.[1]

We focused on the range of molecular motions of the vdW bonded C₆₀ molecules that can be stimulated by the electron beam irradiation. We observed single fullerene's jump in a defective zigzag C₆₀ molecular chain, back and forth translation of a cluster of C₆₀s in a partially filled CNT, pickup of C₆₀ molecules, and rotation of a zigzag chain of C₆₀s accompanied by deformation of the host CNT (Figure 1).

Using a simple model of vdW potential among C₆₀ molecules and the host CNT, we estimated the activation energies for some of the molecular motions, ranging from ~0.3 eV to 0.7 eV (an example is shown in Figure 1). The lowest activation energy is associated with a single C₆₀ detachment at the end of a C₆₀ molecular chain, while the largest activation energy is associated with the molecular jump at a defect site. This demonstrates that molecular vacancies can lead to lower activation energy.

We calculated the probability of electron beam induced breakdown of vdW bonds of C₆₀ molecules. We found that one-dimensional confinement can significantly increase the energy threshold for breaking the bonds. For imaging confined C₆₀s, the optimum electron energy predicted is ~60 kV.

Using above knowledge, we acquired electron diffraction patterns from C₆₀ molecular chains using coherent nanoarea electron diffraction [2-3]. We demonstrated that diffraction peaks from C₆₀ molecules can be recorded when the molecules are ordered and confined in small diameter CNTs. The diffraction patterns coupled with recorded electron images allow us to image the C₆₀ molecules with significantly improved contrast and resolution [4-7].

References

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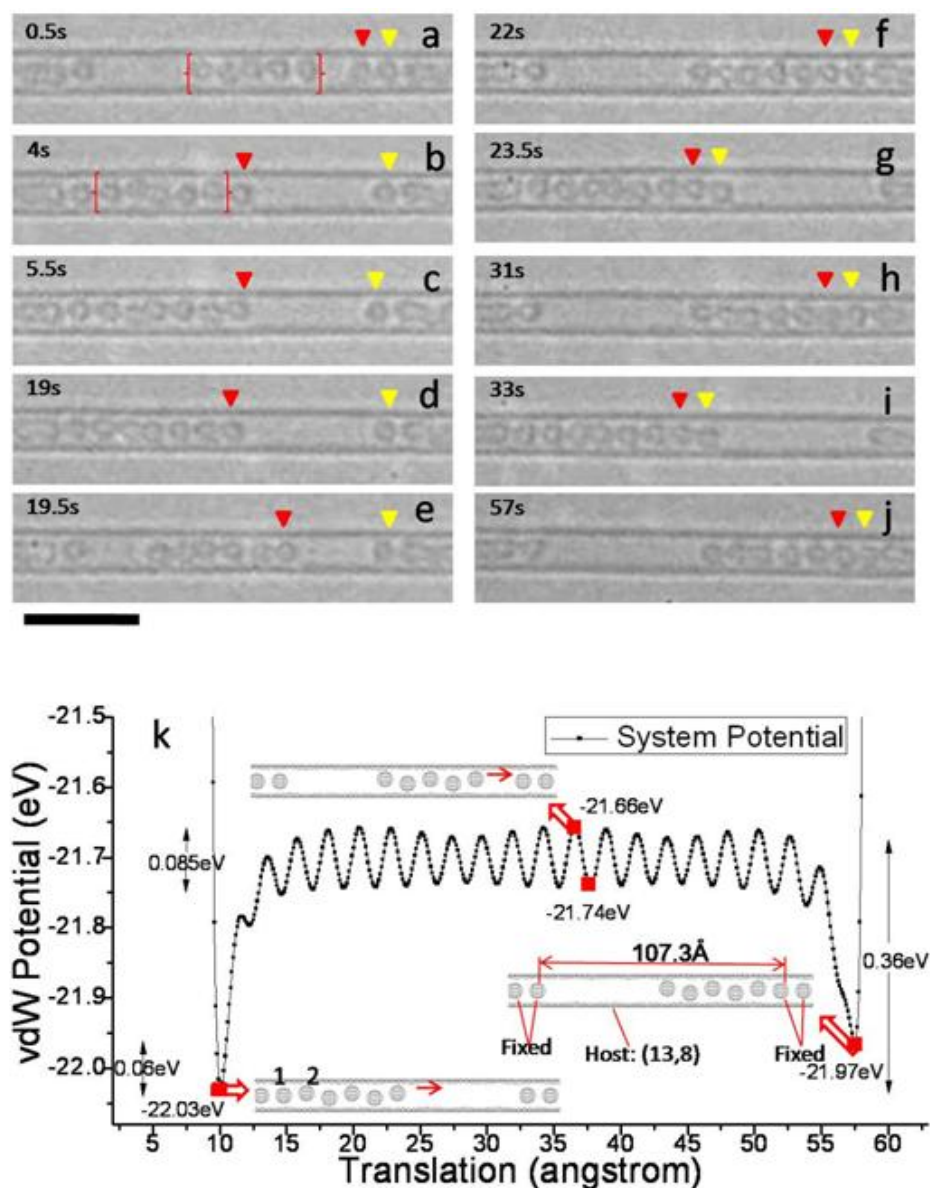


FIG. 1. (a-j) Time series of TEM images captured from a video showing back and forth translations of a small chain of C₆₀s. The recording lasted for 1 min, and 120 frames in total were recorded with an exposure time of 0.5s. The scale bar is 5 nm. (k) Calculated van der Waals potential energy for the translation of a chain of 5 C₆₀s inside a CNT. The structural models used for the calculation is shown in insets for three different positions.