TERAHERTZ MOLECULAR ELECTRONICS USING MINIMUM PROGRAMMABLE MOLECULAR SELF-ASSEMBLED DEVICES

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SUMMARY

Molecular electronics focuses on the development of electronic devices using small molecules with feature sizes in the order of a few nanometers, [Tour, 1998; Derosa, 2002; Wada, 2001; Joachin, 2000; Kwok, 2002] with the ultimate goal of using the minimum amount of atoms for each electronic unit. The fact that the emission and absorption vibrational spectra of most organic molecules are in the terahertz (THz) range showing well localized features in the spatial and energy domains [Seminario, 2002-a] provides the potential of exploiting such a range of the electromagnetic spectrum. In addition, results from on going research have demonstrated the potential use of THz-frequency transmission spectroscopy as a technique for the detection, identification, and characterization of biological agents [Woolard, 2001 & 2002]. A very recent research has demonstrated using sophisticated molecular dynamics simulations the possibility of modulating molecular vibrations that eventually could be able to make signal processing in nanoscopic molecular units [Seminario, 2002-a]. The molecular unit is made of four gold clusters interconnected by four molecules as shown in Figure 1. The interconnecting molecules show negative differential impedance as has been recently demonstrated [Seminario, 2002-b]. Molecules and clusters of 1 nm size cannot be assembled as standard semiconductor devices using modern lithographic techniques. The alternative is the use of techniques such as self-assembly and vapor deposition, which bring a strong random component into the field [Seminario, 2002-c]. Fortunately, these deposition techniques lead to patterns that can eventually be driven to forming specific arrays [Seminario, 2001-a & 2002-d] containing minimum units that can be thoroughly analyzed with the intent of studying their programmable characteristics [Seminario, 2001-a & 2002-e].

To obtain feasible information about the stability of molecular devices that are being proposed as minimum units for building molecular electronic systems, simulations on minimum square units were performed using molecular dynamics simulations with information from precise quantum mechanical calculations. The results of these simulations were analyzed by a time and frequency domain data analysis, using digital signal processing techniques [Seminario, 2002-a], which yielded valuable spectral information regarding the dynamical nature of the molecular units. The molecular units and other structures that may be proposed as basic units to build molecular

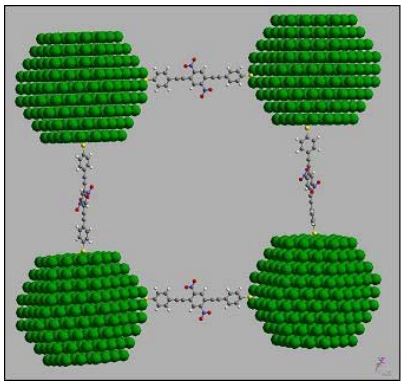

Figure 1. Minimum programmable unit

electronic devices, contain thousands of atoms, such large amount is within the viable range of sizes that can be handled by precise molecular dynamics simulations. The signal processing techniques proposed in this work allowed us to obtain important information, through the use of an alternative viewpoint of the standard vibrational frequencies analysis, which would be difficult for this size of systems. Vibrational behavior of relevant bonds across the molecular unit at several temperatures yields information that complements experimental efforts leading to understand and exploit the intrinsic characteristics of molecular electronic devices as well as to predict their stability at operating temperatures. A detailed analysis of the frequency spectra yields correlations between several local vibrations. If these correlations can be used to include vibrational signals externally introduced into local parts of the molecular device, several single operations can be performed between them thus enabling the possibility of having molecular processors dealing with signals a the THz range of frequencies. Figure 2 shows the particular bond (left) used as example in this abstract. The time dependent

carbon-hydrogen vibration is also shown (center), which does not correspond to a pure vibration but to a modulated signal modified by other vibrational modes. In several cases it was found that the modulating signal corresponds to the gold clusters vibrations, which can be externally excited. Therefore further processing could occur between signals inputted through the gold clusters; therefore, several possibilities are under study in our labs. The development of THz systems has strong connection with future combat systems and with other relevant aspects of the army. Further information can be found in the web site of the Moletronics group at USC (see http://www.ee.sc.edu/research/molectronics)

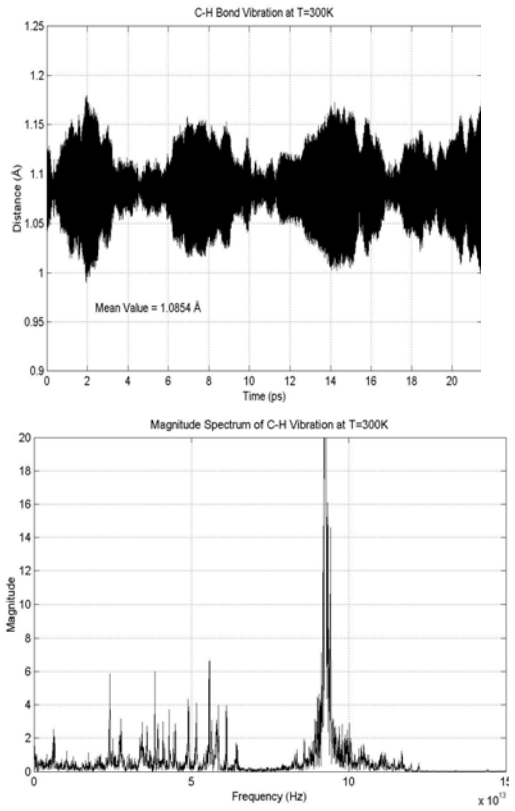

Figure 2. Molecular dynamics simulations at 300 K provide precise information on specific bonds. The carbon-hydrogen (CH) bond in a benzene ring is considered. The time evolution of the carbon-hydrogen distance is shown (upper) for an interval of 20 picoseconds. The corresponding frequency spectrum (lower) shows a central peak at ~90 THz. The widening of this peak and the presence of other peaks are consequence of the interactions with other vibrational modes not related to the CH bond. External signals can be introduced to the gold clusters (Figure 1) and processed in the active molecules.

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