A simple way for the passive THz imaging

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Progress in terahertz (THz) optics and commercial availability of the infrared thermal imaging cameras with thermal sensitivities of 12 to 45 milliKelvins allow putting forward a simple way for the passive imaging the objects-sources of the THz radiation. In the framework of this approach, the THz objective forms the image of the object on the two-dimensional THz radiation-to-heat converter. The converter represents a matrix of the material transparent in the THz wavelength range, with a lot of embedded 9 nm nickel nanoparticles isolated from each other. The nanoparticles being heated by the THz radiation, convert the THz energy to heat. And the two-dimensional pattern being formed by heated nanoparticles in the converter is visualized by the infrared thermal imaging camera. In accordance with the number of pixels and thermal sensitivity of the specific commercial uncooled infrared camera, it is estimated the number of nickel nanoparticles per the element-object of the converter corresponding to the pixel-image.

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Isomeric transition of C10 molecule from star to ring conformations

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Studying the possible path of fullerene formation [1] in arc discharge plasma we have predicted a new metastable star-shaped isomer of the C10 molecule which along with the ring-shaped isomer plays the key role in formation of the C20 fullerene.

There is an open question on the possibility of radiative transition from star to ring conformations of the C10 molecule. To get an answer to this question we have performed quantum chemical calculations on the C10 molecule using the semiempirical molecular orbital PM3 method [2] and the ab-initio plane-wave pseudopotential method (PWscf program of ESPRESSO package [3]). Our calculations show that C10 transition conserves the D5h symmetry of the isomers. Note that conformation transition have been observed for molecules (e.g. the barrier for inversion of the ammonia molecule is 0.2 eV [4]).

By using the PM3 method we have calculated reaction coordinate of the star to ring transition. The corresponding energies for PM3 obtained atomic configurations was calculated also by using PWscf. The ring isomer was found to be lower in energy by 9.39 eV (PM3) and by 12.52 eV (PWscf) than the star isomer. Barrier for transition from the metastable star state to the ring state is 8.41 eV (PM3) and 1.70 eV (PWscf). Energies of E1' type vibrations of the star and ring isomers calculated by the PM3 method are 0.24 eV and 0.08 eV, respectively.

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