

M@C_{2n} N, N-dimethylformamide solutions optical properties

E.K. Alidzhanov¹, Yu.D. Lantukh¹, S.N. Letuta¹, S.N. Pashkevitch¹,
O.A. Domachin¹, I.E. Kareev², V.P. Bubnov², and E.B. Yagubskii²

¹Orenburg State University, 460018 Orenburg, Russia

²Institute of Problems of Chemical Physics RAS, 142432 Chernogolovka, Russia

Endohedral structures are the novel forms of nanomaterials, which hold much promise for practical application. However its physical and chemical properties are little-investigated. In this work the relative photo-physical properties of M@C_{2n} (M = Gd, Ce, La) N,N-dimethylformamide (DMF) solutions and C₆₀ toluene solution (10⁻⁵ M) were investigated by absorption and luminescence spectroscopy. Examined endometallofullerenes were produced by DC electric arc discharge followed by extraction in polar solvents [1].

The visible (400-800 nm) region spectra of endometallofullerenes solutions showed the long absorption tails without any clear absorption peaks. In the UV-region (250-400 nm) absorption spectra of M@C_{2n} solutions, as well as spectra of C₆₀ toluene solution, shows fast growth of absorption ratio with the wavelength decreasing. The M@C_{2n} dominant absorption and luminescence peaks corresponding to HOMO-LUMO transitions are situated at IR-region. Due to different symmetry of HOMO-LUMO molecular orbital such electron transitions are forbidden that why IR-region peaks are ill-defined. We revealed intensive luminescence peaks in 450-600 nm region for M@C_{2n} DMF solutions. Concentration and temperature dependence as well as photoluminescence excitation spectra for these luminescence bands were measured. We found that photoluminescence excitation and absorption spectra of M@C_{2n} solutions has rather different structure. We consider that endometallofullerenes molecules formed nanodimension aggregates in DMF solution and detected luminescence have "solid-state" nature.

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Raman study of diameter-dependent resonance effects and “metallic window” for different types of single-wall carbon nanotubes

S.N. Bokova¹, E.D. Obraztsova¹, A. Kukovecz², M. Smolik², and H. Kuzmany²

¹*Prokhorov General Physics Institute, 119991, 38 Vavilov street, Moscow, Russia*

²*University of Szeged, Rerrich Bela ter 1, H-6720 Szeged, Hungary*

³*University of Wien, Institute of Materialphysics, Strudlhofgasse 4, A-1090, Wien, Austria*

The geometry of single-wall carbon nanotubes (SWNTs) completely defines their electronic structure and conductivity type. SWNTs can be metals or semiconductors with different gap values. It is important to have an instrument being sensitive to this parameter. A resonant Raman spectroscopy has been proved as one of the most informative techniques for such diagnostics. Usually the resonant conditions are provided by variation of laser excitation energy. In our work another approach has been developed: at fixed laser wavelength the resonance conditions were reached via variation of the average SWNT diameter. The Raman spectra have been registered at different excitation energies (14 laser lines) for several sets of HiPCO (high pressure CO decomposition) and arc SWNTs grown with different catalysts. The nanotubes with diameters 0.76-1.41 nm have been revealed in different materials. For excitation energies being resonant for metallic nanotubes the tangential Raman mode is asymmetrically broadened due to the electron-phonon interaction (Fano-resonance).

The metallic Fano-broadening is observed under excitation energies depending on the SWNT diameter. The energy range for “metallic windows” in different nanotubes has been estimated by two methods: Raman scattering and UV-VIS-NIR optical absorption. The results of both techniques have coincided very well.

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Spectral investigations of fullerene-porphyrin complexes and adducts

B. Laskowska¹, B. Barszcz¹, A. Bogucki¹, A. Graja¹, and R.M. Ion²

¹*Institute of Molecular Physics, Polish Academy of Sciences, 60-179 Poznan, Poland*

²*VALAHIA University of Targoviste, 130082 Targoviste, Romania*

The unique shape of the fullerenes C₆₀ and C₇₀ combined with their distinct physical properties make them good candidates for preparation of large, supramolecular aggregates. On the other hand porphyrins with their electronic absorption properties have been widely used as electron-donating species in photoactive molecular dyads. For an enhanced understanding of the chromophore interaction between fullerenes and various porphyrin-derived dyes we have performed spectral studies using both experimental and theoretical methods. These data should be important for design and preparation of the solar energy converters.

The present work reports spectral investigations of some π -oxo-dimers complexes of trivalent metals (Mn, Fe) with two different ligands: tetraphenylporphyrin (TPP) and tetranaphthylporphyrin (TNP), and fullerene (C₆₀ and C₇₀) complexes with π -oxobis[5,10,15,20-tetraarylporphyrinatoiron (III)] (FeTXP)₂O dimer, where X=phenyl or naphthyl and π -oxobis[5,10,15,20-tetraarylporphyrinatomanganese (III)] (MnTPP)₂O dimer, where aryl is phenyl and naphthyl. These complexes have isolated packing of fullerenes in which fullerene molecule is embraced in a pocket built by porphyrins. Molecular configurations of the chromophore molecules and complexes are presented and discussed. The configuration and spectral properties of porphyrin-derived chromophore – fullerene adducts are also given.

Herein we report the UV-Vis-IR absorption studies and Raman scattering investigations of both classes of fullerene-porphyrin systems. Our overall goal is to understand the correlation between the structure of new fullerene-derived systems and their spectral properties recorded in the solid state. An assignment of main electronic and vibrational bands has been made. In order to describe and analyze electronic structure and normal vibrations of the investigated complexes and adducts, the equilibrium geometry, charge distribution and vibrational excitations were calculated with DFT method using appropriate basis.

It was stated that significant charge redistribution occurs in both fullerene and porphyrin moieties upon covalent linkage or complexation. These effects are mainly observed as shifts and/or broadening of both electronic and vibrational bands in comparison with respective free porphyrins and fullerenes features.

Plasmon resonances in fullerene ions

A.K. Belyaev*, V.K. Ivanov⁺, R.G. Polozkov⁺, A.S. Tiukanov*, A.I. Toropkin*,
A.V. Solov'yov[#], and W. Greiner[#]

*Herzen University, Moika 48, 191186 St.Petersburg, Russia

⁺St. Petersburg State Polytechnic University, Politechnicheskaya 29, 195251 St.Petersburg,
Russia

[#]Frankfurt Institute for Advanced Studies, Johann Wolfgang Goethe University, Robert-Mayer
Str. 10, D-60054 Frankfurt am Main, Germany

The photoionization cross sections of the fullerene C₆₀ and its positive ions C₆₀^{q+} (q=1,2,3) are calculated within the photon energy range from the ionization thresholds up to 80 eV and compared with the recent experimental data [1] and other calculations for C₆₀⁺. The main attention is paid the giant plasmon resonance in photoabsorption.

The calculations are performed within the Local Density Approximation. The basic Kohn-Sham equations are used for determining of the single-electronic wave functions. The calculations are performed within the jellium model for positive core for both the sphere and the spherical layer: valence electrons are considered in the averaged field of 60 ions of C⁺⁴ [2]. In the present work the theoretical approach is improved by means of using the Perdew-Wang parametrization for the exchange-correlation energy functional.

The phototransition amplitude of each orbital is calculated both within the single-electron approximation and also by taking into account many-electron correlations within the Random Phase Approximation. The total photoionization cross section is calculated as a sum of partial cross sections for each orbital.

The calculated photoionization cross sections for the neutral fullerene, as well as for its ions indicate the giant plasmon resonances with positions of ~20 eV for all fullerenes. The physical nature of the resonances is discussed. This is in a good agreement with the classical Mie theory and the experimental data [1] for the ions C₆₀⁺, C₆₀²⁺ and C₆₀³⁺. The analysis shows that the dominant contribution in the giant resonance for the total cross sections is due to the ionization from the 6g and the 5f shells with some contribution from the 4d and 2s shells. The photoionization cross sections calculated in the present work fulfill the sum rule for all fullerenes under the consideration, so in contrast to the previous calculations [2] they are not scaled by any factor.

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Photophysics and quantum chemical simulation of organic conjugated structures doped with nanoobjects: effect of the charge transfer complex formation

N.V. Kamanina¹ and E.F. Sheka²

¹Vavilov State Optical Institute, 12, Birzhevaya Line, 199034 St.-Petersburg, Russia

²People's Friendship University of the Russian Federation, 117921 Moscow, Russia

An active interest has been taking in photophysics and quantum chemical simulation of organic π -conjugated systems doped with nanoobjects (such as fullerenes, nanotubes, nanoparticles, *J*-aggregates, nanofibers, etc.) due to their exclusive linear and nonlinear optics, dynamics and structural features [1,2]. These can be exploited as effective optical limiters, modulators and laser beam switchers. Different mechanisms, promoting the action, can be activated, among which there are reverse saturable absorption, laser-induced change in the refractive index, carrier free absorption, complex formations, etc. Nanoobject insertion stimulates the media self-organization as well as an increase in the polarizability and order parameters that results in the formation of quasi-photonic organic systems. Figure 1 shows one of such quasi-photonic systems based on polyimide, when Si-based and quartz substrates have been used.

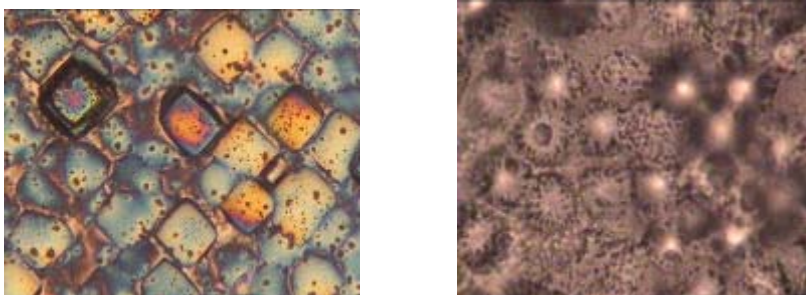


Figure 1. Quasi-photonic organic crystals observed in π -conjugated polymer materials doped with nanotubes.

The present paper is devoted to the consideration of the charge transfer complex formation between polyimides presenting the conjugated organic medium on one hand and either fullerene C₆₀ or single-wall nanotubes (SWNTs) on the other hand. The effect of the complex formation on the photorefractive and optical limiting properties of the composites has been discussed. Semiempirical quantum chemical calculations have been performed for two binary systems, both involving a triphenylamine fragment of polyimides as the composite donor component and either fullerene C₆₀ or 14-layer (4, 4) SWNT as acceptor component. Both experimental findings and calculation results point to a wide area of feasible optoelectronics application of these systems treated at 532, 805, 1047, 1064, 1315, 1500, 2940 nm. Moreover, these structures are fairly promising for applications in medicine, biology and display technique.

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Photophysics and quantum chemical simulation of organic conjugated structures doped with nanoobjects: structures and interface conditions

N.V. Kamanina¹, E.F. Sheka², L.A.Chernozatonskii³, A.I. Vangonen¹,
P.Ya. Vasilyev¹, and Yu.M. Voronin⁴

¹Vavilov State Optical Institute, 12, Birzhevaya Line, 199034 St.-Petersburg, Russia

²People's Friendship University of the Russian Federation, 117921 Moscow, Russia

³Institute of Biochemical Physics, RAS, 19991 Moscow, Russia

⁴State Institute of Fine Mechanics and Optics, 197101 St. Petersburg, Russia

Last decade the switching characteristics of multilayer electrooptical structures based on oriented nematic liquid crystal (NLC) doped with fullerene-containing charge-transfer complexes or nanotubes have been intensively studied. The new way to improve the switching parameters of the electrooptical systems is to treat the transparent conducting layers or nanotubes relief with surface electromagnetic waves [1]. As the results, the conductivity of the systems can be enhanced, the laser stability of the conducting layer can be improved, the value of the applied voltage can be decreased and the switching parameters can be changed from millisecond time range to microsecond one.

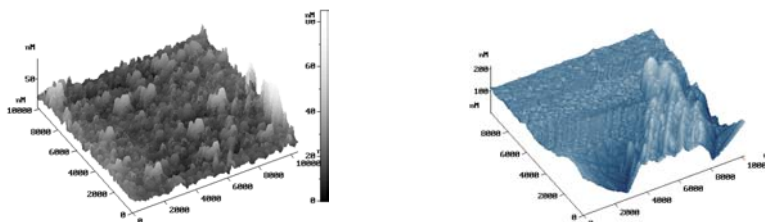


Figure 1. AFM image of the interface modified with nanotubes. The figures present nanotube relief before (*first*) and after (*second*) treatment with surface electromagnetic wave.

The present paper is concentrated on the interaction between nanotubes themselves which leads to their coalescence and gives rise to changing the anisotropy at the interface between a solid and electrooptical mesophase. As turned out, the tube coalescence makes the switching in the electrooptical materials, that is characteristic for, say, liquid crystals, more effective and fast. Semiempirical quantum chemical calculations have been performed for a dyad of 14-layer (4, 4) SWNTs. Intermolecular interaction (IMI) between the tubes involves a considerable contribution of the donor-acceptor interaction since the donor and acceptor efficiencies of any carbon SWNT look like those of fullerene C_{60} . DA-burdened IMI results in a multi-well structure of the ground state IMI term that, in its turn, distinguishes two regions of the intermolecular shortest contacts, corresponding to either a coalescent pair at short distances or weakly interacting tubes which form a charge transfer complex at longer distances. The two states are separated by a barrier that well explains features of the experimental techniques which provide SWNTs adhesion. Characteristics of the coalescent pair are compared with those of individual tubes. Expected changes caused by replacing sole tubes by coalescent compositions and concerned with electrooptical properties of the devices are discussed.

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Injection of electrons from different nanocarbon electrodes at the moderate cathodic potentials

N.S. Komarova and A.G. Krivenko

Institute of Problems of Chemical Physics, RAS, 142432 Chernogolovka, Moscow Region, Russia

The electrochemical behavior of electrodes containing nanotube carbon materials of different morphology (nanopaper, nanotubes of particular structure with the length from 0.5 to 3 mm, nanostructure consisting of long parallel columns of about 50 nm in a diameter) has been studied.

The intensive dark-blue coloration hexamethylphosphoric triamide (HMPA) solution was obtained for different nanocarbon electrodes at the moderate cathodic potentials ($\lambda \sim -1.2$ V). Electron spin resonance spectrum of dark-blue frozen HMPA solution consisted of single narrow line having $\Delta H = 0.58$ mT and $g = 2.0024$ coincided with $g_e = 2.0023$. Similar effects have earlier been observed on smooth metallic electrodes but at far cathodic potential range ($\lambda \sim -3.5$ V). Dark-blue coloration was caused by emission of electrons into HMPA solution [1, 2]. Thus obtained results unambiguously prove injection of electrons at interface of nanocarbon structure/solution at the moderate cathodic potentials.

Fotoemission work function has earlier been demonstrated to arcwise decrease at potential shift to cathodic region [3]. However the dependence of injection current on λ does not obey the Fowler-Nordheim equation in HMPA solution but it has power character with exponent ~ 2.5 . Similar conformity was observed in other electrolytes.

Thus injection of electrons was shown to occur at the moderate cathodic potential region relative to smooth metallic electrodes from nanocarbon structures into electrolyte solution. Application of carbon nanostructures permits to use of high reactive solvated electrons for electrochemical activation of a stable compounds.

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Spectroscopic testing of nanocarbon fluids as molecular photoprobes for DNA molecules

O. Kysil^{*+}, I. Sporysh^{*}, E. Buzaneva^{*}, U. Ritter⁺, and P. Scharff⁺

^{*}*Radiophysics Faculty, Taras Shevchenko National University of Kyiv, Volodymyrska str. 64, 01033 Kyiv, Ukraine*

⁺*Institut für Physik/FG Chemie, TU Ilmenau, D-98684 Ilmenau, Germany*

Nanocarbon photoprobes are nanofluids, which contain water-suspended carbon nanotubes or fullerene molecules, functionalised by oxygen, hydroxyl or carboxylic groups. Their controlled strong photoresponse at visible range depends from electronic features of biomolecular surrounding [1]. Therefore designed nanofluids are proposed for molecular diagnostics in biological liquids.

Previously designed nanocarbon fluids [2, 3] are tested (using UV-visible-NIR, IR and PL spectroscopies) for molecular detecting of single and double stranded DNA molecules, with or without induced defects. Analysis of experimental data shows effect of PL wavelength and intensity changing in aqueous biological media as a response to structural modifications of various DNA molecules. These testify PL spectroscopy of nanocarbon fluids as informative method of examination of photostimulated nanocarbon behavior in biomolecular surrounding, also as nanocarbon fluids as perspective biological molecular photoprobes.

Based on the experimental results the proposed models of photoinduced processes at interface between functional groups and carbon nanotubes or fullerene molecules, also as functionalized nanocarbons and tested molecules, are presented.

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Raman scattering of multi-walled carbon nanotubes with the structural defects

Î .P. Dmytrenko¹, N.P. Êulish¹, L.À. Êî marova¹, S.V. Lizunova¹, N.Ï . Belyi¹, Yu.À. Grabovskiy¹, V.À. Gubanov¹, L.A. Bulavin¹, Yu.I. Prylutsky², and L. Valkunas³

*Kiev National Shevchenko University, Departments of Physics¹ and Biophysics²,
Vladimirskaya Str., 64, 01033 Kiev, Ukraine*

*³Institute of Physics, Laboratory of Molecular Compounds Physics, Savanoriu, 231,
LT-02300 Vilnius, Lithuania*

In view of the special features of their structure carbon nanotubes (CNT) possess a number of unique properties. Depending on changes in their structure the transformations of the vibrational and electron structure of CNT take place. The influence of structural defects on different properties of CNT is studied less. In particular, the appearance of a D Raman scattering band, and also its two-phonon contribution (D* band), caused by scattering phonons on the boundary of Brillouin zone, is typical for the CNT. Presence of a D band is caused by the removal of prohibition on the appearance of this scattering because of the disordering of the crystalline structure, caused by the presence of defects, in particular, the boundaries of fine dispersed grains. Analogously, the two-phonon scattering, whose intensity can even exceed its value for the forbidden D band, is determined by the contribution of the structural defects of CNT.

Usually, above both bands for the multi-walled CNT are compared in the intensity with the permitted G band and change form, broadening, intensity in the dependence on the synthesis conditions of CNT and external action. It is important to determine the type of defects and the nature of their influence on the Raman scattering bands indicated. In this work, on the basis of the assumption, that the defectiveness of CNT depends on correlation in the arrangement of their separate layers, α and β parameters of the deformation and twin packing defects were studied. The analysis of the broadening of X-ray diffraction reflections from the CNT is carried out and the probabilities of the disturbances in the layer packing, which are compared with the nature of changes in the Raman scattering bands, are determined.

It is important to note, that disturbance in the layer packing, the sizes of the blocks of coherent scattering, the microstresses, obtained as a result of the high-energy electron irradiation, are accompanied by reconstruction of the scattering bands, connected with the structural defects. In this case the asymmetry, broadening and intensity of these lines, which consist of different contributions and correlate with different types of defects, are changed.

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Spin-dependent stages of free charge carriers photogeneration in molecular complexes of fullerene C₆₀ with organometallic donors

D.V. Lopatin*, V.V. Rodaev*, D.V. Konarev⁺, and R.N. Lyubovskaya⁺

*Tambov State University, 392000 Tambov, Russia

⁺Institute of Solid State Physics RAS, 142432 Chernogolovka, Russia

Layered molecular complexes of fullerene C₆₀ with cadmium diethyldithiocarbamate and coordination monomer formed by zinc diethyldithiocarbamate and ligand hexamethylenetetraamine: (Cd(Et₂dtc)₂)₂*C₆₀ (**1**) and (Zn(Et₂dtc)₂*HMTA)₂*C₆₀ (**2**) are characterized by significant photoresponse magnitude ($\sim 10^3$). It makes **1** and **2** promising materials for the design of novel photodetectors. Thus, transfer and transformation of electronic excitation energy in these crystals is an actual problem.

We have studied intermediate stages of free charge carriers photogeneration in **1** and **2** by means of magnetic field effects (MFEs) analysis.

For **1** the relative change of the photoconductivity excited by white light was saturated at induction of MF $B \sim 0.3$ Oe attaining the value -4%. In the case of **2** the field dependence was characterized by saturation at $B \sim 0.1$ T with the effect magnitude 1%. The different features of MFEs indicate various mechanisms of the influence of MF on the photoconductivity of **1** and **2**.

MF is capable to change the interaction rate constant of triplet (T) CT-excitons with trapped charges leading to their release. A collision of the triplet CT-exciton with paramagnetic species (R) with multiplicity $M=2$ may occur either spin-independent triplet scattering or quenching. The rate constant (Q) of quenching depends on the amplitude of the doublet component in the intermediate pair (T...R). At $B=0$ the doublet component is uniformly distributed over all six spin states of (T...R) and the value of Q is maximum. MF reduces the number of spin states possessing the doublet component. It results in the decrease of Q and the photoconductivity of **1** as a consequence.

Since lifetimes of singlet (S) and triplet CT-excitons are unequal MF modulates their common concentration inducing S-T intercombination transitions due to the difference of g-factors of ionic states forming CT-excitons. It leads to an increase of the probability of dissociation of CT-excitons into free charge carriers and an enhancement of photoconductivity of **2** as a result.

Revealed various magnetosensitive stages of free charge carriers photogeneration in **1** and **2** indicate the possibility of controlling fullerene-based materials' photoelectric properties via spin degrees of freedom.

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Comparative Raman study of the C₆₀H₃₆ and C₆₀H₆₀ fullerene hydrides

K.P. Meletov¹, I.O. Bashkin¹, V.V. Shestakov¹, I.I. Tartakovskii¹,
A.A. Maksimov¹, J. Arvanitidis², D. Christofilos², and G.A. Kourouklis²

¹*Institute of Solid State Physics RAS, Chernogolovka, Moscow region 142432, Russia*

²*Physics Division, School of Technology, Aristotle University of Thessaloniki, GR-54 124 Thessaloniki, Greece*

The Raman spectra of C₆₀H₃₆ and C₆₀H₆₀ prepared under high hydrogen pressure are measured at ambient conditions. The C₆₀H₃₆ samples were obtained from pristine C₆₀ by its treatment at a hydrogen pressure of 3 GPa and T=620 K during 25 h, and the C₆₀H₆₀ samples were synthesized at P_{H₂}=5 GPa and variable temperatures, T=620–770 K, during 26.5 h. The hydrogen quantity during hydrogenation was always excessive and corresponded to a ratio H/C₆₀=90–120. The hydrogen contents in the final products were determined by combustion in the oxygen flow and weighing the combustion products, H₂O and CO₂.

The Raman spectrum of C₆₀H₃₆ includes over 120 sharp peaks whereas only 17 peaks were observed on C₆₀H₆₀ (Fig.1). A large number of the phonon peaks in the spectra of hydrogenated fullerenes is related to the lowered symmetry of these molecules compared to pristine C₆₀. The symmetry lowering results in splitting of the degenerate modes and lifting of the symmetry restrictions in the Raman scattering. Moreover, the C₆₀H₃₆ products consist of several isomers that have different phonon frequencies. The C₆₀H₆₀ molecule does not seem to have isomeric forms; accordingly, its Raman spectrum is less abundant. The important feature of both spectra is the C-H stretching modes in the range 2800-3000 cm⁻¹. The frequencies of these modes show a large isotopic shift when protium is substituted with deuterium.

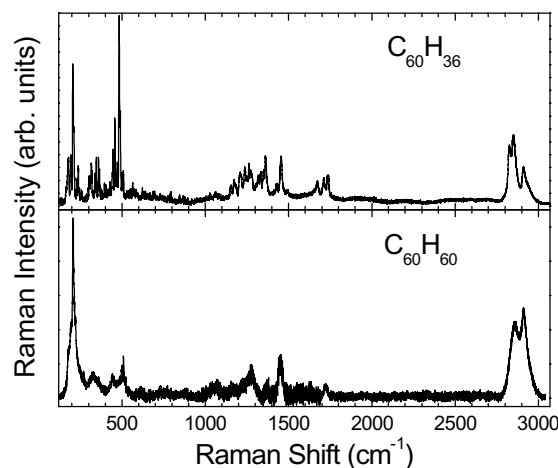


Figure1. Raman spectra of C₆₀H₃₆ and C₆₀H₆₀ at ambient conditions.

Both materials show high luminescence in the visible spectral range that is more intense for C₆₀H₆₀. To avoid screening of the Raman signal by the luminescent background, we used the 676.4 nm Ar⁺ laser line for the Raman measurements.

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Superposition of quantum and classical rotational motions in $\text{Sc}_2\text{C}_2@C_{84}$

K.H. Michel¹, B. Verberck¹, M. Hulman^{2,3}, H. Kuzmany², and M. Krause^{2,4}

¹*Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, 2020 Antwerpen, Belgium*

²*Institut für Materialphysik der Universität Wien, Wien, Austria*

³*ARC Seibersdorf Research GmbH, A-2444 Seibersdorf, Austria*

⁴*Institute for Ion Beam Physics and Materials Research, Forschungszentrum, Rossendorf, PF510119, D-01314, Dresden, Germany*

The superposition of the quantum rotational motion (tunneling) of the encapsulated Sc_2C_2 complex with the classical rotational motion of the surrounding C_{84} molecule in a powder crystal of $\text{Sc}_2\text{C}_2C_{84}$ fullerite is investigated by theory. Since the quantum rotor is dragged along by the C_{84} molecule, any detection method which couples to the quantum rotor (in casu the C_2 bond of the Sc_2C_2 complex) also probes the thermally excited classical motion (uniaxial rotational diffusion and stochastic meroaxial jumps) of the surrounding fullerene. The dynamic rotation-rotation response functions in frequency space are obtained as convolutions of quantum and classical dynamic correlation functions. The corresponding Raman scattering laws are derived, the overall shape of the spectra and the width of the resonance lines are studied as functions of temperature. The results of the theory are confronted with experimental low-frequency Raman spectra on powder crystals of $\text{Sc}_2\text{C}_2C_{84}$ [1]. The agreement of theory with experiment is very satisfactory in a broad temperature range [2].

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Oligomers $(\text{Pt}_{0,75}\text{C}_{60})_n$ as the electron acceptor in polymer solar cells

D.S. Martyanov^{*}, V.V. Bruevich^{*}, E.M. Nechvolodova⁺, Yu.N. Novikov[†],
M.V. Tsikalova[†], and D.Yu. Paraschuk^{*}

^{*}*Faculty of Physics & International Laser Center, Lomonosov Moscow State University,
Moscow 119992, Russia*

⁺*Nesmeyanov Institute of Organoelement Compounds, 119991 Moscow, Russia*

[†]*Semenov Institute of Chemical Physics, 119991 Moscow, Russia*

Fullerenes and their derivatives in blends with conjugated polymers are well known to be the most effective acceptors for photoinduced charge transfer reaction. In addition, fullerenes in these blends can form a highly conductive network for collection of photoinduced charges (electrons) making fullerenes indispensable in bulk-heterojunction polymer solar cells. However, the active layer of such a cell comprises about 80% of fullerene, which almost does not absorb the solar light. In this work, we study a recently synthesized fullerene-based coordination polymer $(\text{Pt}_{0,75}\text{C}_{60})_n$ as an acceptor for bulk-heterojunction solar cells. $(\text{Pt}_{0,75}\text{C}_{60})_n$ could facilitate electron transport in the bulk heterojunction allowing decreasing the fullerene content in it. Moreover, such a polymer is expected to influence phase separation peculiarities, which are very important for the device performance. We have investigated donor-acceptor composites of poly[2-methoxy-5-(2'-ethyl-hexyloxy)-1,4-phenylene vinylene] (MEH-PPV) with $(\text{Pt}_{0,75}\text{C}_{60})_n$ using photoluminescence, photoinduced absorption spectroscopy, and photoelectric methods. The properties of MEH-PPV/ $\text{Pt}_{0,75}\text{C}_{60}$ blends are compared with those of MEH-PPV/ C_{60} .

Optical absorption spectra of MEH-PPV/ $\text{Pt}_{0,75}\text{C}_{60}$ composite indicate the absence of essential donor-acceptor interaction of the components in the electronic ground state. We have observed that $(\text{Pt}_{0,75}\text{C}_{60})_n$ strongly quenches MEH-PPV photoluminescence (PL). For both acceptors strong PL quenching was observed at less than 0.01% acceptor content. We have found that PL quenching at acceptor content $\approx 10\%$ is more efficient in MEH-PPV/ C_{60} blends. This could be due to lower electron affinity of $(\text{Pt}_{0,75}\text{C}_{60})_n$ or/and more pronounced phase separation in MEH-PPV/ $\text{Pt}_{0,75}\text{C}_{60}$ blends as compared with C_{60} . However, at higher acceptor content, the PL quenching efficiencies in both blends are very similar. Current-voltage characteristics under white illumination and photocurrent action spectra of bulk-heterojunction MEH-PPV: $\text{Pt}_{0,75}\text{C}_{60}$ photodiodes are measured and compared with those of MEH-PPV: C_{60} ones. Photoinduced charge generation and charge transport in MEH-PPV: $\text{Pt}_{0,75}\text{C}_{60}$ composites are discussed.

Optical properties of the \tilde{N}_{60} and \tilde{N}_{70} fullerene films, alloyed by oxygen with the annealing

Î. P. Dmytrenko¹, N.P. Êulish¹, E.L. Pavlenko¹, N.M. Belyi¹, Yu.I. Prylutsky², U. Ritter³, and P. Scharff³

*Kiev National Shevchenko University, Departments of Physics¹ and Biophysics²,
Vladimirskaya Str., 64, 01033 Kiev, Ukraine*

³Institute of Physics, Technical University of Ilmenau, D-98684 Ilmenau, Germany

The oxidation of fullerenes, as is known, leads to the degradation of many properties, characteristic for their condensed state, which realizes in the form of molecular broadband semiconductor crystals. The fullerite doping, connected with the filling of interstitial positions, causes special interest with the oxidation, since in this case the formation of fullerene-oxygen compounds is possible. However, the nature of intermolecular interaction in such systems is studied insufficiently. The calculation of the transfer of charges between the oxygen atoms and C_{60} molecules shows, that in contrast to other alloying elements, the doping with oxygen leads to the oxidation processes with the transfer of electrons from fullerenes to the impurities. The hybridization of electronic states in this case is insignificant. From other side, with the accumulation of the oxygen molecules in the fullerites, their molecular states substantially change, about which the transformation of interband electron transitions with the annealing testifies. At the same time, the vibrational spectra change little, although with an increase in the annealing time the growth of the Raman scattering background is observed, i.e., the accumulation of defects on the frame of fullerenes takes place. In this work a study of changes in the behavior of vibrational modes, electronic and crystal structure of the C_{60} and C_{70} fullerene films with their prolonged annealing is carried out. Annealing was conducted at a temperature of 473 K during from 5 to 20 h. The vibrational spectra were investigated by the Raman scattering method, the electron transitions were studied by the photoluminescence method and spectral ellipsometry, and the crystal structure was determined with the use of X-ray diffractometry.

With an increase in the annealing time the insignificant splitting of H_g modes in the C_{60} fullerenes, and also the separate peaks of the Raman scattering of the C_{70} molecules, are observed, although the C_{70} fullerenes react to the presence of oxygen less. The effects of decrease in the $A_g(2)$ peaks, characteristic of polymerization, are not observed, although their asymmetry is noticeable. The photoluminescence spectra both in the region of the basic peak, connected with the emission of Frenkel's excitons on the dimeric traps, and near the additional maximums undergo essential transformations. The noticeable transformation of the optical conductivity spectra occurs in the entire range of energies, including the ultraviolet interval. The intensity of the Raman scattering peaks decreases with the long times of annealing, and its background grows. For the C_{70} fullerites the special features indicated are observed too, but they are substantially slowed.

Thus, the oxidation of the crystalline phase of fullerites is connected not only with the ionization of components, but also with the noticeable hybridization of electronic states, which leads to the degradation of fullerenes, although its extent differs for the C_{60} and C_{70} molecules.

Spectral evidence of low symmetry of C₆₀ fullerene and its derivatives

B.S. Razbirin¹, E.F. Sheka², E.A. Nikitina³, A.N. Starukhin¹, D.K. Nelson¹,
M.Yu. Degunov¹, P.A. Troshin⁴, and R.N. Lyubovskaya⁴

¹*Ioffe Physical-Technical Institute RAS, St. Petersburg, 194021 Russia*

²*Peoples' Friendship University of the Russian Federation, Moscow, 117923 Russia*

³*Photochemistry Center RAS, Moscow, Russia*

⁴*Institute of Problems of Chemical Physics RAS, Chernogolovka, 142432 Russia*

Conventionally, the I_h symmetry of fullerene C₆₀ is accepted that is a widely spread basic standpoint for numerous studies devoted to the interpretation of the molecule electronic spectra (see review [1] and references therein). Discussions are mainly concentrated on the lowest $S_0 \leftrightarrow S_1$ transitions, strictly forbidden by symmetry within the I_h point group. However, the detailed examination of both electronic (absorption and fluorescence) and vibrational (Raman scattering and IR absorption) spectra have revealed a set of peculiarities, such as a weak 0_0^0 transition in both absorption and fluorescence spectra, the vibronic series in the latter spectrum based on g -symmetry vibrations, absolutely allowed pattern of the phosphorescence spectrum, the "silent" modes in Raman and IR spectra, and others, which are inconsistent with the high symmetry of the molecule and cast some suspicion on the point. But numerous calculations, persistently declaring the I_h symmetry, have been shutting off the "green light" to the suspicions. Practically, all available calculation techniques have been applied to the molecule making the statement concerning its I_h symmetry quite immovable. Nevertheless, it has recently been shown that the conclusion is resulted from the consideration of the molecule electron system, of its odd electrons in particular, in a close-shell approximation without taking the electron spin into account [2]. Passing to the open-shell approximation has lead to the symmetry lowering up to C_i . The detailed analysis performed in [2] in the framework of the Hartree-Fock approach, has shown that the symmetry of the pure spin singlet state of the C₆₀ molecule cannot be higher than C_i . The finding has made us to revise the electronic spectra interpretation.

Experimental data considered in the current paper involve fluorescence and absorption spectra of the molecule in the toluene solution recorded at room and low (80, 2K) temperatures. Additionally to fullerene C₆₀, a set of its derivatives, such as aziridinofullerene (C₆₀NH), two fulleropyrrolidines (1-methyl-3,4-FP and 1-methyl-2(4-pyridyl)-3,4-FP), and ethyl ester of fullerenoacetic acid (C₆₀CHCOOCH₂CH₃), have been studied in view of the effects caused by the addends of different structure on the fullerene core. Simultaneously, the calculations of both equilibrium structures in the ground state (UHF version of the AM1 semiempirical technique) and excited states spectra (one-point ZINDO/S calculations) have been performed. As for fullerene C₆₀, the symmetry lowering explains naturally all qualitative symmetry-characterizing features mentioned above. As for quantitative characteristics, the latter are to evidently depend on the quantitative measure of the symmetry deviation. As shown in [2], the symmetry lowering from I_h to C_i results in the average change of the C-C bond length dispersion from 0.001 to 0.02 Å. According to the obtained ZINDO/S results, these changes turned out to be not sufficient to lift the $S_0 \leftrightarrow S_1$ transition oscillator strength keeping it at the zero value. When going to derivatives, the deviation of the fullerene core structure becomes more severe and causes, firstly, the onset of the allowed-like electron transition pattern of the aziridinofullerene spectra, which further becomes much more pronounced for other species. The calculated and experimental results fit each other perfectly well. The work was supported by the RFBR (gr. 07-03-00755).

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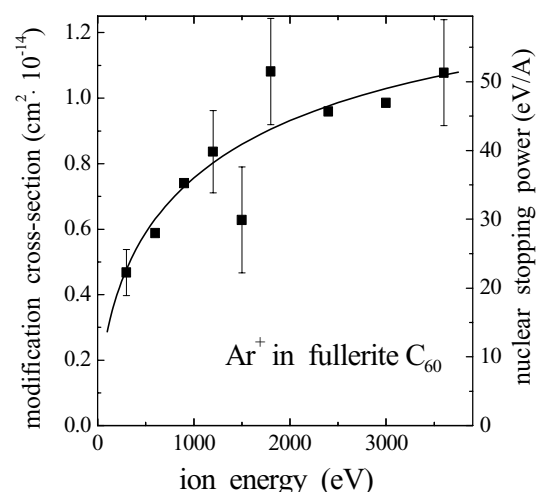
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The role of ion cascades in amorphization of fullerite C₆₀ by Ar⁺ ions and in forming the image of ion nano-probe

V.V. Shnitov, V.M. Mikoushkin, and Yu.S.Gordeev

Ioffe Physical-Technical Institute RAS, St.-Petersburg, 194021 Russia

Ion lithography is becoming an effective tool in nanotechnologies due to significant progress in developing ion nano-probes. Since fullerite could be used as an ion resist with extremely small grains, knowledge about interaction of ions with fullerite C₆₀ films is of importance. Unfortunately this information is scanty contrary to that in the field of ion collisions with single fullerenes in the gas phase [1-2]. Mechanisms of defect creation, modification and, finally, amorphization of fullerite by Ar⁺ ion beams in the keV energy range have been studied in this research. As a result of the amorphization, insoluble and non-evaporable lithographic image of ion probe was created. The modification process was controlled by electron energy loss spectroscopy (EELS) by measuring both the density of states in the band gap [2] and intensities of the molecular peaks in loss-spectra. The first criterion characterizes the extent of amorphization and the second one points to the extent of destruction of fullerene molecules. Dependences of these criteria on the dose of ion irradiation allowed determination of the rates and absolute cross-sections of amorphization and fullerene destruction. Cross section of fullerene destruction proved to be essentially larger than that of defect creation. This fact evidences for chemical reactions between “kick out atoms” and small fragments resulting in reparation of broken bonds after ion-fullerene collision. The cross sections of the ion-induced modifications proved to be about geometric section of fullerene, which confirms the result of [1]. It means that one Ar⁺ ion radically destroys fullerene in collision. The conclusion was made that it can be possible due to generation of cascade of secondary carbon ions in the fullerene aggregates. Figure shows energy dependences of cross-section of fullerene destruction (points) and nuclear stopping power of Ar⁺ ion in graphite (solid line) corrected for the fullerite density. Coincidence of these dependences (to the scaling factor) evidences the mechanism of fullerene destruction due to quasi-elastic atomic collisions without electron excitations and fullerene heating. Analysis of nuclear stopping power showed that the cascade dimension does not exceed the area of three fullerenes in the keV-energy range. Consequently, the image of ion nano-probe in fullerite resist should not essentially exceed the probe size in the keV energy range despite the crucial role of cascades of secondary ions. The research was supported by the Russian Academy of Sciences (P-03, N2-2-14) and by INTAS (06-1000012-8972).



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Electrical properties and photovoltaic effect in n-Si/fullerite C₆₀ and n-Si/nanocomposite C₆₀:Cu heterostructures

D.M. Spoiala

*“Superconductivity and Magnetism” Laboratory, Moldova State University,
60 A. Mateevici Str., Chisinau, MD-2009, Moldova*

Thin films of fullerite C₆₀ (d~0.1–0.5 μm) and C₆₀:Cu nanocomposite (NC) (d~0.05–0.5 μm) were deposited using the method of thermal evaporation in vacuum. The substrates of n-type crystalline Si wafers (ρ=4.5 Ω·cm) and quartz for electrical measurements and NaCl single crystals for transmission electron microscopy examination were used. The current-voltage (I-V) characteristics of n-Si/C₆₀ and n-Si/C₆₀:Cu heterostructures at different temperatures in darkness as well as under light illumination were measured.

Typical I-V dark characteristics of n-Si/C₆₀ heterostructure exhibit strong rectification properties. The rectification ratio for best sample reaches the value of $3.3 \cdot 10^4$ at ±2 V. The detailed analysis of forward and reverse branches of I-V characteristics is performed.

Under light illumination of the n-Si/C₆₀ heterostructure a photovoltaic effect is observed. At light intensity of 20 mW/cm² at room temperature we obtained U_{oc}=0.201 V, J_{sc}=14.67 μA/cm² and fill factor FF=0.198. The low values of obtained parameters usually are attributed to the high series resistance of the device (R_s~10⁴ Ω) which is due to high resistivity of fullerite C₆₀ films. Therefore, it is natural to assume a decrease resistivity of fullerite C₆₀ films. One of the ways is obtaining nanocomposite C₆₀: metall thin films in which metal nanoparticles are uniformly dispersed in fullerite C₆₀ matrix.

The electrical resistivity of C₆₀:Cu NC thin films deposited on quartz were 10⁴-10⁵ Ω·cm at room temperature. The temperature dependence of conductivity in 291-403 K range was typical for semiconductor for all samples with two different slopes on σ-1/T curve. The conduction mechanisms of NC thin films are discussed.

The n-Si/C₆₀:Cu heterostructure, like n-Si/C₆₀, shows rectification properties with ratio 10-200 at ±2V for different samples. At light illumination the photovoltaic effect also is observed. At intensity of 20 mW/cm² we obtain U_{oc}=0.24 V, J_{sc}=241.1 μA/cm² and FF=0.225. In this way, an increase of main parameters of photovoltaic device is performed.

The spectral responses of both heterostructures in 400-900 nm spectral ranges were investigated.

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Dynamics of clusters radiating defects generation in silicon

N.Yu. Suchkova and A.A. Dmitrievskii

Tambov State University by G.R. Derzhavin, Tambov, 392600 Russia

Some decades silicon is the basic material in microelectronics. Apparently, the nearest years the situation cardinally will not change. At the same time, silicon becomes a constructional material for micromachines, sensor controls, micro- and nanoelectromechanical systems (MEMS/NEMS). Therefore, even the little changes of its mechanical properties induced by various external factors, become important, and their studying - actual. Electrical and mechanical properties of silicon strongly depend on qualitative and quantitative structure of radiating defects (RD) and them clusters.

In work the dynamics of radiating defect clusters generation in conditions of low-flux electron irradiation was investigated.

Single-crystals of Si n- and p-type were investigated. A ^{90}Y - ^{90}Sr radioactive sources with intensity $I=10^5 \text{ ? } 3 \cdot 10^6 \text{ cm}^{-2}\text{s}^{-1}$ was used to irradiate the samples. As the basic characteristic the value of microhardness H has been chosen.

The exposition of samples in a field of beta-particles leads to nonmonotonic change of microhardness. The forming of the inprint can be carried out due to: movements of dislocations, phase transitions under indenter and mobility of nonequilibrium point (radiating) defects. Dislocations in silicon at room temperatures are motionless. Before [1], it was revealed that the phase transitions under the indenter did not affect irradiated unhardening. Hence, nonmonotonic dependence of microhardness on time of an irradiation is connected with multistage process of a point (own and radiating) defects subsystem transformation.

The results received by independent methods (isochronal annealing at different stages of irradiation, research of dependence of H changes speed from intensity of irradiation, and also synchronous researches of changes H and concentrations of electrical-active RD by DLTS methods), have allowed to identify of the defects clusters dominating at different stages of irradiation. The first maximum of unhardening is associated with accumulation of clusters, consisting of two vacancies, atom of oxygen and atom of carbon. On the stage of repeated unhardening the dominate clusters including interstitial and substitutional atoms of carbon and/or interstitial atoms of carbon and oxygen. The qualitative model of quasichemical reactions which products are specified clusters is offered.

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Singlet oxygen generation processes in solutions of fullerenes in carbon tetrachloride

I.V. Bagrov, I.M. Belousova, O.B. Danilov, A.V. Ermakov, A.S. Grenishin,
V.M. Kiselev, I.M. Kislyakov, T.D. Murav'eva, E.N. Sosnov, and
D.A. Videnichev

The singlet molecular oxygen generation is studied by means of its NIR luminescence at the light excitation by pulse, pulse-periodic and CW sources in C_{60} and C_{70} solutions in CCl_4 . The singlet oxygen concentration is determined in the stationary and pulse regimes of irradiation. The quenching rate constants of $^1\Delta_g$ state of O_2 molecule by fullerene are found to be $(7.2 \pm 0.1) \cdot 10^7 \text{ M}^{-1}\text{s}^{-1}$ (\tilde{N}_{70}) and $< 6 \cdot 10^4 \text{ M}^{-1}\text{s}^{-1}$ (\tilde{N}_{60}). Temperature and photolytic changes in the solutions photosensibilization ability are studied using optical and ESR spectroscopy methods. A pulse liquid singlet oxygen generator is constructed and studied on the base of the C_{60} solution in CCl_4 .

Production of the singlet oxygen into gas phase is realized with the concentration $5 \cdot 10^{16} \text{ cm}^{-3}$.

Optical and photoelectrical properties of fullerene-Zn(II)tetraphenylporphyrin complex

I.B. Zakharova*, E.A. Donenko*, Yu.F. Biryulin⁺, and L.V. Sharonova⁺

* State Polytechnic University, St. Petersburg, 195251 Russia

⁺Ioffe Physical-Technical Institute RAS, St. Petersburg, 194021 Russia

Fullerene-porphyrin dyads and complexes have been the subject of intense research as artificial systems, which efficiently process solar energy [1-3]. In this work the interaction of these molecular components, optical and photoelectrical properties of C₆₀-Zn(II)tetraphenylporphyrin (C₆₀-ZnTPP) thin films has been investigated extensively.

The films were formed by the method of vacuum evaporation in quasi-closed volume on different substrates. Optimal technological parameters of the complex manufacturing with different composition are discussed. The dissociation temperature of this charge-transfer complex into the molecular components at vacuum deposition is higher than that of C₆₀-mesotetraphenylporphyrin (C₆₀-H₂TPP) [4]. Initial studies of condensation and surface morphology of the films are investigated by AFM and SEM methods. Optical absorption spectra in UV, visible and IR regions are studied. The origin of additional absorption line in complex films at 800-850 nm is discussed.

Photoluminescence spectra at 300 and 80 K of the both ZnTPP and C₆₀-ZnTPP films have been measured. The main peak ZnTPP at 1.90 eV is not shifted by formation of the complex, but the positions of the other peaks strongly depend on temperature and complex composition. The experimental results are explained on the basis of *ab initio* calculations [4]. Non-linear optical properties of C₆₀-ZnTPP complex are predicted.

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Photoluminescence and structure of fullerite C₆₀ intercalated with hydrogen

I.V. Legchenkova, N.B. Silaeva, Yu.E. Stetsenko, K.A. Yagotintsev,
P.V. Zinoviev, and V.N. Zoryansky

*Verkin Institute for Low Temperature Physics and Engineering, 47 Lenin Ave., Kharkov
61103, Ukraine*

Fullerite C₆₀ as a wide gap (~2eV) semiconductor, is a promising material for electrotechnical applications (sun cells, FET's, LED's, etc). However unlike conventional semiconductors, charge transport characteristics of C₆₀ depend strongly on the molecular orientational state. The aim of this work was to study how the orientational state in of the C₆₀ lattice can be controlled by intercalating it with gases with small van der Waals radii. The structural and optical properties of C₆₀ intercalated with molecular hydrogen were studied using the X-ray powder diffraction and spectral luminescence methods. X-ray diffraction studies yielded data on the influence of the intercalation conditions on the structural characteristics, the orientational phase transition, and the orientational vitrification temperatures of C₆₀ crystals. The spectral luminescence studies in temperature region 5-300K have shown that the whole photoluminescence spectrum broadens and shifts towards lower energies under H₂ intercalation. The changes in the spectrum are presumably due to emission centers, which appear around dopant molecules and which are perturbed Frenkel excitons delocalized over the nearest neighbor shell of C₆₀ molecules. The intercalation related mechanism the formation of such luminescent centers is discussed. The temperature dependence of the integrated luminescence intensity dependence suggests that presence of H₂ molecules in interstitial voids of the *fcc* C₆₀ lattice increases the orientational glass formation temperature. The latter is, most likely, associated with changes in the interaction between C₆₀ molecules and it is an important factor which appreciably affects the electric and luminescent properties of fullerite C₆₀.