Final report
Project NK 105691
Science in nanolaboratories

Participants:

Péter Matus and Gyöngyi Klupp left the project because they took positions outside Hungary. Zsolt Szekrényes and Katalin Németh obtained positions outside academia. They were replaced by Hajnalka Tóháti, who has expertise in spectroscopy, and later Dávid Földes, who was promoted from student to participant status based on his expertise in sample preparation. Hajnalka Tóháti left the project in the beginning of 2017 but stayed in the research group. Students involved were Dávid Földes (MOF synthesis), Bence Szabados (fullerene synthesis and spectroscopy) and Judit Horváth (spectroscopy of fulleride salts).

Work plan:

We could not buy the planned liquid handling system, because our investment budget was cut by 16M HUF. Therefore we could prepare far less metal-organic frameworks than originally planned. This affected the structural and spectroscopic work and shifted it towards nanotubes as containers.

We present the results organized by topic (molecular containers, molecules, encapsulated systems, other hybrid systems and additional topics) and give the list of publications in the end, in order to be able to refer to them in the text. In case of unpublished work (including unpublished conference posters and theses) we present the results in a more detailed form.

Molecular containers

Our results on carbon nanotubes concerned their chemical reactivity towards sidewall functionalization. We showed that for solid-state reactions in small diameter tubes, the standard rule of increasing reactivity with decreasing diameter does not hold, due to bundling effects [A-11,T-2].

In boron nitride nanotubes, we determined the purification procedures from commercial material and studied the defect structure by near-field infrared spectroscopy with 20 nm spatial resolution. We employed these tubes as containers for fullerene molecules [A-21,C-22,C-27,T-6].

We determined the structures of several coordination compounds, related to metal-organic frameworks (MOFs) by single crystal X-ray diffraction in collaboration with various Hungarian research groups [A-9,A-15, A-24, A-25, A-26]. We started our MOF studies with molecular crystals of related monomers. To study the supramolecular properties of MOFs, we also developed and optimized the synthesis of various fullerene cocrystals of basic Zn-benzoate [C-9,C-14,C-23,T-4]. We developed a new family of six new MOFs with Zn-based secondary building units (SBUs) and 1,4-cubanedicarboxylate linkers [C-19,C-25,C-26,T-8]. We

successfully prepared the (RS)spiro[3.3]heptane-2,6-dicarboxylic acid containing analogue of MOF5 with high symmetry structure similar to the original MOF5 material. For further experiments, we synthesized racemic spiroheptane in large amounts. As the synthetic work took longer than expected, the publication of these results in articles will follow in the next months.

Molecules

We performed model calculations connected to structural studies on nanoparticles. The most sophisticated measurements of such nature will be conducted at free-electron laser x-ray sources. We showed that if a very intense x-ray pulse causes a sample to undergo Coulomb explosion, then by measuring the spatial distribution of the fragments it is possible to determine the initial orientation of the cluster [A-1]. Further, we started to develop a new method for the determination of particle shape, from a single diffraction pattern. This type of experiments and theoretical developments can be integrated into our work on the structure of particles in the nanolaboratories [A-5].

As an example of small structures built from simple organic molecules, we studied microdot and microrod formation during pentacene oxidation [A-23]. The formation and transformations of supramolecular systems were studied in uracil-based molecules connected by hydrogen bonds. Temperature-dependent infrared spectra, complemented by density functional theory (DFT) computations, proved that in different temperature ranges different intermolecular forces were dominant (H-bonds, van der Waals interactions and π-π stacking) that resulted in structural phase transitions [A-22,T-1].

Other possible encapsulated systems are based on linear carbon chains. We performed model calculations on linear polyenes from short oligomers to polyacetylene, to determine their bond lengths and electronic structure, comparing the approach from molecular orbitals to that of energy bands. These two approaches showed excellent agreement [A-27,C-17,C-24].

Fullerene derivatives are often used for insertion of functional groups into nanocontainers. These molecular adducts have to be characterized thoroughly in order to predict their behavior in an encapsulated system. For this purpose, we determined the structure of an anthracene derivative of the fullerene C_{60} [A-3]. Another molecular family with very exciting properties is the one of fulleride anions [A-6,C-5]. Clusters and solids based on these building blocks can show intriguing properties and phase transitions as metallicity, superconductivity and magnetism, opening new perspectives when put into nanolaboratories. Our most important results in this area concerned the investigation of the phase diagram of expanded superconducting fulleride salts of the composition $Cs_xRb_{(3-x)}C_{60}$, a series of isostructural materials exhibiting varying chemical pressure in the crystal. Thus a pressure-temperature space was constructed and various physical properties studied in wide international collaboration. Our own results, obtained by temperature-dependent infrared spectroscopy, underlined the metal-insulator transition through the coupling of electrons and molecular vibrations. We identified a new phase between the metallic and insulating structure, which we termed "Jahn-Teller metal". Starting from this phase and lowering the temperature, a special non-BCS superconducting state is obtained. We published these results in Science Advances and the paper also gained substantial publicity in the popular science press [A-12,C-2,C-4,C-5,C-6,C-12,C-13,C-18,T-9]. In Li_4C_{60} we presented evidence from infrared

spectra for the intermolecular bonds between fullerenes and also concluded that there is no metallic electronic conductivity present in this material. These findings underlined the description of Li_4C_{60} as a polymeric ionic conductor [A-16].

Silicon carbide (SiC) nanoparticles are very promising candidates as emission centers in host-guest hybrids. We were able to demonstrate a switching mechanism in the luminescence correlated with the size of particles. Our most important result is that the relatively strong and broad luminescence in molecular-sized SiC nanoparticles of 13 nm is related to surface chemical groups instead of quantum confinement. These findings imply that the direction to achieve higher luminescence is chemical modification instead of simple size reduction [A-8]. Size-dependent charge transfer can also be exploited to engineer uniformly sized SiC nanocrystals [A-19]. Another possible added function to SiC nanostructures is energy transfer, resulting in photocatalysis [A-18]. The prospective use of these nanocrystals in nanolaboratories is based on the fact that the size of the crystals can be determined by the external cage (e.g. the diameter of nanotubes).

Encapsulated structures

The smallest nanolaboratories, endohedral fullerenes, consist of few-atom clusters in fullerene cages. We performed structural and spectroscopic studies on face-centered cubic $Sc_3N@C_{80}$, and its cocrystals with various solvents. We determined the rotational dynamics of both the Sc_3N cluster and the C_{80} cage as a function of temperature in these materials [A-2,C-21,T-7].

We continued with a detailed study on the interaction of coronene with various low-dimensional carbon-based structures: single- and multiwalled nanotubes of various diameter and graphite. We showed that both inside and outside the tubes, the coronene molecules undergo polymerization reactions, forming ribbons both outside and inside and inner nanotubes inside [A-4,C-1,C-3, C-11,C-20,T-3]. Further we showed that encapsulated luminophores can keep their luminescence in single- and double-walled carbon nanotubes. A fullerene-based Eu(III) complex ion pair was filled into nanotubes from supercritical carbon dioxide, thus preserving both the chemical functionality and the optical properties. The encapsulation was proven by infrared and luminescence spectroscopy and transmission electron microscopy [A-7]. In this case, the fullerene was used as a transport “vehicle” to help the chemically attached functional group enter the nanotubes; this method paves the way for introducing other functionalities into nanolaboratories.

Boron nitride nanotubes are a promising alternative to carbon nanotubes due to their insulating character and optical transparency. They can also be used as bases for nanolaboratories, but the encapsulated species behave differently in the two cases. We performed a detailed investigation of fullerene encapsulation into boron nitride nanotubes and found the process to be reversible, i.e. the fullerene molecules could be easily removed from the interior of the tubes. The transparency of the tube wall also helps to follow phase transitions and chemical reactions inside the nanolaboratory. A special product of such a reaction is a carbon nanotube within a boron nitride shell, a shielded cable on the nanoscale [A-21].

Other hybrid systems

New and exciting hybrid structures have been recently discovered based on lead halide perovskites ($CH_3NH_3PbI_3$). We proved that hybrids prepared from $CH_3NH_3PbI_3$ and carbon nanotubes undergo a reversible charge transfer photoreaction which can be followed by infrared and Raman microspectroscopy. Devices fabricated from such structures by our collaborators show unprecedented responsivity as photodetectors [A-17]. We studied the light-induced charge transfer between $CH_3NH_3PbI_3$ and carbon nanotubes, using the carbon nanotube as both transparent layer and charge detector. From the change in the optical spectra in the nanotubes we determined the time scale of the charge transfer process and proved that the mechanism of molecular reorganization (a slow process) is present beside the photoinduced charge generation (fast process) [A-20,C-15].

Another promising solar cell material is amorphous silicon and here the chemical structure also plays a seminal role. We determined the microscopic structure and dynamics of hydrogenated amorphous silicon by infrared microspectroscopic methods. Our nanolaboratories in this case are blisters containing hydrogen on the surface of silicon. We showed that the –SiH groups on the surface form polysilane chains upon annealing, impairing the performance of photovoltaic devices based on aSi:H [A-10].

The treatment at high pressure of the rotor-stator compound C_{60}-cubane, resulted in various new phases with special properties, an ordered superhard structure up to 45 GPa and a fully disordered, but still superhard three-dimensional amorphous network obtained by prolonged treatment at 45 GPa [A-28].

Methodology

We also conducted fundamental studies concerning structure determination methods. We developed an experimental apparatus for the measurement of the Kossel line patterns, which contain not only the magnitude of the scattered waves but also the phase of Bragg reflections. We did two series of experiments at the European Synchrotron Radiation Facility where we obtained very precisely the Kossel line patterns of several samples. We used a setup developed in our home laboratory [A-13,A-14]. We could describe the line profiles of the Kossel pattern of GaAs. We also tested a new detecting scheme for this measurement (the imaging plate) that would open the way to measure Kossel patterns at X-ray free electron lasers by a single pulse, allowing structure determination of various phases existing at extremely nonambient conditions.

Possible exploitation

Although the project has generated exclusively basic science results, some of the effects discovered may be useful for further exploitation. One is the photoluminescence of encapsulated molecules, opening the way to producing light sources on the nanoscale in agressive environments; the other is a possibility of shielded wires consisting of conducting and insulating layers, a first step leading to coaxial cables in nanoelectronics. The potential of the high-pressure derived phases of cubane-fullerene systems as superhard materials is also significant.

Outreach

We published three articles in *Fizikai Szemle*, the monthly journal of the Eötvös Loránd Physical Society, with a broad audience including physics teachers and high-school students. Two of our papers, one on the Jahn-Teller metal state and one on the boron nitride-carbon nanotube, received coverage in the press, in Hungary and abroad.

List of publications resulting from the project:

Articles in international journals:

A-1. Z. Jurek, G. Faigel: **Orienting single-molecule diffraction patterns from XFELs using heavy-metal explosion fragments**
EPL-Europhysics Letters **101,** 16007-1-4 (2013), 1 independent citation

A-2. G. Bortel, É. Kováts, E. Jakab, S. Pekker: **Solvent-free $Sc_3N@C_{80}$-I_h and its precursor cocrystal with toluene**
Fullerenes, Nanotubes and Carbon Nanostructures **23**, 557-565 (2014)

A-3. G. Bortel, É. Kováts, G. Oszlányi, S. Pekker: **Crystal structure of the 4 + 2 cycloadduct of photooxidized anthracene and C_{60} fullerene**
Acta Crystallographica Section E-Structure Reports Online **70,** 444-446 (2014)

A-4. B. Botka, M.E. Füstös, H. M. Tóháti, K. Németh, G. Klupp, Zs. Szekrényes, D. Kocsis, M. Utczás, E. Székely, T. Váczi, G. Tarczay, R. Hackl, T.W. Chamberlain, A.N. Khlobystov, K. Kamarás**: Interactions and chemical transformations of coronene inside and outside carbon nanotubes**,
Small **10**, 1369-1378 (2014), 10 independent citations

A-5. G. Faigel, Z. Jurek: **Particle orientation from distribution of explosion fragments in XFEL experiment**
Acta Crystallographica **A70,** C295 (2014)

A-6. K. Kamarás K, Klupp G: **Metallicity in fullerides**
Dalton Transactions **43,** 7366-7378 (2014), 4 independent citations

A-7. L. Maggini, M.E. Füstös, T.W.Chamberlain, C.Cebrián, M. Natali, M. Pietraszkiewicz, O. Pietraszkiewicz, E. Székely, K. Kamarás, L. De Cola, A. N. Khlobystov, D. Bonifazi: **Fullerene-driven encapsulation of a luminescent Eu(iii) complex in carbon nanotubes**
Nanoscale **6**, 2887-2894 (2014), 4 independent citations

A-8. D. Beke, Zs. Szekrényes, Zs. Czigány, K. Kamaras, A. Gali: **Dominant luminescence is not due to quantum confinement in molecular-sized silicon carbide nanocrystals**
Nanoscale **7,** 10982-10988 (2015), 11 independent citations

A-9. P. Buglyó, K. Lénárt, M. Kozsup, A.C. Bényei, É. Kováts, I. Sóvágó, E. Farkas: **$[Pd(en)(H_2O)_2]^{2+}$ and $[Pd(pic)(H_2O)_2]^{2+}$ complexation by monohydroxamic acids: A solution equilibrium and solid state approach**
Polyhedron **100,** 392-399 (2015)

A-10. C. Frigeri, M. Serényi, Zs. Szekrényes, K. Kamarás, A. Csik, N.Q. Khánh: **Effect of heat treatments on the properties of hydrogenated amorphous silicon for PV and PVT applications**
Solar Energy **119,** 225-232 (2015), 1 independent citation

A-11. K. Nemeth, E. Jakab, F. Borondics, H.M. Tóháti, Á. Pekker, M. Bokor, T. Verebélyi, K. Tompa, S. Pekker, K. Kamarás: **Breakdown of diameter selectivity in a reductive hydrogenation reaction of single-walled carbon nanotubes**
Chemical Physics Letters (618), 214-218 (2015), 1 independent citation

A-12. R.H. Zadik, Y. Takabayashi, G. Klupp, R.H. Colman, A.Y. Ganin, A. Potočnik, P. Jeglič, D. Arčon, P. Matus, K. Kamarás, Y. Kasahara, Y. Iwasa, A.N. Fitch, Y. Ohishi, G. Garbarino, K. Kato, M.J. Rosseinsky, K. Prassides: **Optimized unconventional superconductivity in a molecular Jahn-Teller metal**
Science Advances **1,** e1500059-1-9 (2015), 20 independent citations

A-13. G. Bortel, G. Faigel, M. Tegze, A. Chumakov: **Measurement of synchrotron-radiation-excited Kossel patterns**
Journal of Synchrotron Radiation **23,** 214–218 (2016)

A-14. G . Faigel, G. Bortel, M. Tegze: **Experimental phase determination of the structure factor from Kossel line profile**
Scientific Reports **6,** 22904-1-9 (2016)

A-15. P.L. Parajdi-Losonczi, A.C. Bényei, É. Kováts, I. Timári, T.R. Muchova, V. Novohradsky, J. Kasparkova, P. Buglyó: **[(η^6-pcymene) $Ru(H_2O)_3$]$^{2+}$ binding capability of aminohydroxamates — A solution and solid state study**
Journal of Inorganic Biochemistry **160,** 236-245 (2016)

A-16. D. Quintavalle, B.G. Márkus, A. Jánossy, F. Simon, G. Klupp, M.A. Győri, K. Kamarás, G. Magnani, D. Pontiroli, M. Riccò: **Electronic and ionic conductivities in superionic Li_4 C_{60}**
Physical Review B **93,** 205103-1-8 (2016)

A-17. M. Spina, B. Náfrádi, H.M. Tóháti, K. Kamarás, E. Bonvin, R. Gaal, L. Forró, E. Horváth: **Ultrasensitive 1D field-effect phototransistors: $CH_3NH_3PbI_3$ nanowire sensitized individual carbon nanotubes**
Nanoscale **8,** 4888-4893 (2016), 11 independent citations

A-18. D. Beke, K. Horváth, K. Kamarás, A. Gali: **Surface-mediated energy transfer and subsequent photocatalytic behavior in silicon carbide colloid solutions**
Langmuir **33,** 14263-14268 (2017)

A-19. D. Beke, G. Károlyházy, Zs. Czigány, G. Bortel, K. Kamarás, A. Gali: **Harnessing no-photon exciton generation chemistry to engineer semiconductor nanostructures**
Scientific Reports **7,** 10599-1-6 (2017)

A-20. H.M. Tóháti, Á. Pekker, P. Andričević, L. Forró, B. Náfrádi, M. Kollár, E. Horváth, K. Kamarás: **Optical detection of charge dynamics in $CH_3NH_3PbI_3$/carbon nanotube composites**
Nanoscale **9,** 17781-17787 (2017)

A-21. K.E. Walker, G.A. Rance, Á. Pekker, H.M. Tóháti, M.W. Fay, R.W. Lodge, C.T. Stoppiello, K. Kamarás, A.N. Khlobystov: **Growth of carbon nanotubes inside boron nitride nanotubes by coalescence of fullerenes: Toward the world's smallest coaxial cable**
Small Methods **1,** 1700184-1-9 (2017)

A-22. Zs. Szekrényes , P.R. Nagy, Gy. Tarczay, L. Maggini, D. Bonifazi, K. Kamarás: **Direction-dependent secondary bonds and their stepwise melting in a uracil-based molecular crystal studied by infrared spectroscopy and theoretical modeling**
Chemical Physics Letters **691,** 163-168 (2018)

A-23. A.Ž. Tomović, J.J. Savić, N.Lj. Bakić, G. Bortel, G. Faigel, R. Zikic, V.P. Jovanović: **Oxidized pentacene micro-rods obtained by thermal annealing of pentacene thin films in air**
Vacuum **144,** 36-42 (2017)

A-24. F. Matyuska, A. Szorcsik, N.V. May, Á. Dancs, É. Kováts, A. Bényei, T. Gajda: **Tailoring the local environment around metal ions: a solution chemical and structural study of some multidentate tripodal ligands**
Dalton Transactions **46,** 8626-8642 (2017)

A-25. N. Marozsán, H. Horváth, É. Kováts, A. Udvardy, A. Erdei, M. Purgel, F. Joó: **Catalytic racemization of secondary alcohols with new (arene)Ru(II)-NHC-tertiary phosphine complexes**
Molecular Catalysis **445,** 248-256 (2018)

A-26. P. Buglyó, I. Kacsir, M. Kozsup, I. Nagy, S. Nagy, A.C. Bényei, É, Kováts, E. Farkas: **Tuning the redox potentials of ternary cobalt(III) complexes containing various hydroxamates**
Inorganica Chimica Acta **472,** 234-242 (2018)

A-27. S. Pekker: **From methyl radical to polyacetylene: Size-dependent structural properties of linear polyenes**
Journal of Nanoscience and Nanotechnology, accepted Dec. 18, 2017 (2018)

A-28. M. Du, M. Yao, B. Sundqvist, P. Ge, Q. Dong, É. Kováts, S. Pekker, S. Chen, R. Liu, B. Liu, T. Cui, B. Liu: **New ordered structure of amorphous carbon cluster induced by fullerene-cubane reactions**
Advanced Materials, accepted Feb. 12, 2018 (2018)

Conference presentations:

C-1. K. Kamarás, H.M. Tóháti, G.Klupp, K. Németh, B.Botka, R. Hackl, M.E. Füstös, T.W. Chamberlain, A.N. Khlobystov: **Hybrid materials formed from coronene and carbon nanostructures**
Materials Research Society 2013 Fall Meeting, Boston, MA, USA, November 2013, poster

C-2. G. Klupp: **Jahn-Teller evidence in fulleride IR spectra**
ICTP-LEMSUPER Conference "Mechanisms and developments in light-element based and other novel superconductors", Trieste, Italy, September 2013, invited lecture

C-3. K. Kamarás: **Hybrid materials formed from carbon nanostructures and organic molecules**
International workshop "From carbon nanotubes to graphene: the key materials to the future?", Universitá Cattolica del Sacro Cuore, Brescia, Italy, September 2013, invited lecture

C-4. K. Kamarás, J. Horváth, G. Klupp, V. Kocsis, I. Kézsmárki, A.Y. Ganin, M.J. Rosseinsky, R. Colman, R.H. Zadik, M.D. Tzirakis, Y. Takabayashi, K. Prassides: **Dynamic Jahn-Teller effect in IR spectra of expanded Cs_3C_{60} fullerides at low temperature**
XXIInd International Symposium on the Jahn-Teller Effect, Graz, Austria, August 2014, lecture

C-5. J. Horváth, G. Klupp, K. Kamarás: **Jahn-Teller effect in C_{60}^{3-} studied by infrared spectroscopy in solution**
XXIInd International Symposium on the Jahn-Teller Effect, Graz, Austria, August 2014, poster

C-6. G. Klupp, J. Horváth, P. Matus, K. Kamarás, V. Kocsis, I. Kézsmárki, A.Y. Ganin, M.J. Rosseinsky, R.H. Colman, R.H. Zadik, M.D. Tzirakis, Y. Takabayashi, K. Prassides: **The parent magnetic Mott-Jahn-Teller state of the high-T_c Cs_3C_{60} superconductor studied by infrared spectroscopy**
5th EuCheMS Chemistry Congress, Istanbul, Turkey, September 2014, lecture

C-7. K. Kamarás: **Infrared spectroscopy and microscopy on nanostructures**
Astromineralogy Workshop II, Konkoly Observatory, Budapest, Hungary, September 2014, lecture

C-8. K. Kamarás: **Cloaking of Encapsulated Molecules in Carbon Nanotubes at Infrared Frequencies**
6th Szeged International Workshop on the Advances in Nanoscience, Szeged, Hungary, October 2014, lecture

C-9. É. Kováts, G. Bortel, G. Oszlányi, D. Földes, S. Pekker: **New MOFs with cubane based linkers**
6th Szeged International Workshop on the Advances in Nanoscience, Szeged, Hungary, October 2014, poster

C-10. G. Faigel: **New uses of an old method the x-ray diffraction**
Workshop on Ultrafast processes in Photosystems, New vistas at ELI ALPS, Szeged, Hungary, 2014 October 18-21, invited lecture

C-11. K. Kamarás, M.E. Füstös, B.S. Nagy, E. Székely, T.W. Chamberlain, A.N. Khlobystov: **Encapsulation of organic molecules in carbon nanotubes from supercritical carbon dioxide**
Hungarian Conference on Supercritical Fluids 2015, Budapest University of Technology and Economics, May 2015, lecture

C-12. G. Klupp, P. Matus, R.H. Zadik, R.H. Colman, Y. Takabayashi, M.J. Rosseinsky, K. Kamarás, K. Prassides: **Emergence of the Jahn–Teller metallic state in alkali metal fullerides shown by infrared spectroscopy**
The 11th International Symposium on Crystalline Organic Metals, Superconductors and Magnets (ISCOM2015), Bad Gögging, Germany, September 2015, poster

C-13. K. Kamarás, G. Klupp: **Symmetry, Jahn-Teller effect and unconventional solid-state phenomena in fulleride salts**
International Conference „Athene's Chemistry", honoring Prof. Magdolna Hargittai, Budapest University of Technology and Economics, November 2015, lecture

C-14. D. Földes: **New metal organic frameworks with the incorporation of cubane** *International Joint Conference on Enviromental and Light Industry Technologies, International Symposium on Design and Innovative Technologies, Budapest, November 2015, poster*

C-15. Á. Pekker, H.M. Tóháti, Zs. Szekrényes, K. Kamarás, E. Horváth, M. Spina, B. Náfrádi, L. Forró: **Photochemical studies on CH3NH3PbI3 - carbon nanotube hybrids**
International Conference "From Solid State to Biophysics VII: From Basic to Life Sciences", Cavtat, Croatia, June 2016, lecture

C-16. K. Kamarás, Á. Pekker, H.M. Tóháti, B. Botka, K.E. Walker, A.N. Khlobystov, R. Hackl, Y. Nishimura, H. Witek, S. Irle: **Cloaking of encapsulated molecules in carbon nanotubes at infrared frequencies**
Seventeenth International Conference on the Science and Application of Nanotubes and Low-Dimensional Materials - NT16, Vienna, Austria, August 2016, lecture

C-17. S. Pekker: **From benzene to graphene: oligomers and polymers of trigonal carbon**
Seventeenth International Conference on the Science and Application of Nanotubes and Low-Dimensional Materials - NT16, Vienna, Austria, August 2016, poster

C-18. K. Kamarás, G. Klupp, P. Matus, M.J. Rosseinsky, K. Prassides: **Optical signatures of the Jahn-Teller metal state in fulleride superconductors**
XXIIIrd International Symposium on the Jahn-Teller Effect, Tartu, Estonia, August 2016, lecture

C-19. É. Kováts, G. Bortel, E. Jakab, S. Pekker: **New high-symmetry layered cocrystal of tetranuclear zinc benzoate**
30th Meeting of the European Crystallographic Association, Basel, Switzerland, August 2016, poster

C-20. K. Kamarás, B. Botka, B.S. Nagy, M.E. Füstös, G. Klupp, H.M. Tóháti, E. Székely, T.W. Chamberlain, A.N. Khlobystov: **Graphene nanoribbon formation inside carbon nanotubes**
European Physical Society CMD26 Conference, Groningen, The Netherlands, September 2016, lecture

C-21. J. Horváth, É. Kováts, G. Bortel, S. Pekker, K. Kamarás: **Vibrational spectroscopy of endohedral fullerenes revisited**
European Physical Society CMD26 Conference, Groningen, The Netherlands, September 2016, poster

C-22. K. Kamarás, Á. Pekker, A. Szám, H.M. Tóháti, K.E. Walker, G.A. Rance, A.N. Khlobystov: **Encapsulated molecules in boron nitride nanotubes**
7th Szeged International Workshop on the Advances in Nanoscience, Szeged, Hungary, October 2016, invited lecture

C-23. É. Kováts: **New family of Zn carboxilate MOFs with cubane linkers**
7th Szeged International Workshop on the Advances in Nanoscience, Szeged, Hungary, October 2016, lecture

C-24. S. Pekker: **From benzene to graphene: oligomers and polymers of trigonal carbon**
7th Szeged International Workshop on the Advances in Nanoscience, Szeged, Hungary, October 2016, poster

C-25. D. Földes, É. Kováts, G. Bortel, E. Jakab, S. Pekker: **MOF-5 analogue structures with cubane**
7th Szeged International Workshop on the Advances in Nanoscience, Szeged, Hungary, October 2016, poster

C-26. D. Földes, É. Kováts, G. Bortel, S. Pekker: **New zinc carboxylate-based metal-organic frameworks with cubane-1,4-dicarboxylic acid linkers**
4th European Crystallography School (ECS4), Warsaw, Poland, July 2017, poster

C-27. D. Datz, G. Németh, Á. Pekker, K.E. Walker, G.A. Rance, A.N. Khlobystov, K. Kamarás: **Nano-spectroscopy of phonon-polariton modes in boron nitride nanostructures**
33rd European Conference on Surface Science, Szeged, Hungary, August 2017, poster

C-28. K. Kamarás: **Nano-containers and nano-scaffolds**
AE-ALLEA-YAE joint Conference 2017, Budapest, Hungary, September 2017, lecture

Student theses connected to the project:

T-1. Zsolt Szekrényes: **Study of complex nanostructures by infrared spectroscopy**
PhD, Óbuda University, 2015
T-2. Katalin Németh: **Chemical modification and optical spectroscopy of single-walled carbon nanotubes**
PhD, University of Pannonia, 2016
T-3. Bea Botka: **Optical and Raman spectroscopy of carbon nanotube-based hybrid materials**
PhD, Budapest University of Technology and Economics, 2016

T-4. Dávid Földes: **Preparation and investigation of metal-organic frameworks**
MSc, Eötvös Loránd University, 2015
T-5. Gergely Németh: **Investigation of nanostructures by near-field infrared spectroscopy**
MSc, Budapest University of Technology and Economics, 2016
T-6. Dániel Datz: **Near-field infrared nanospectroscopy**
MSc, Eötvös Loránd University, 2016
T-7. Judit Horváth: **Investigation of carbon-based nanostructures by infrared spectroscopy**
MSc, Budapest University of Technology and Economics, 2017

T-8. Dávid Földes: **High-symmetry fullerene cocrystals**
BSc, Eötvös Loránd University, 2015
T-9. Judit Horváth: **Investigation of fulleride anions by infrared spectroscopy**
BSc, Eötvös Loránd University, 2015
T-10. Bence Szabados: **Investigation of molecular thin films by infrared spectroscopy**
BSc, Eötvös Loránd University, 2017

Seminars and colloquia:

[S-1] June 21, 2013 – Johannes Kepler University, Linz, Austria, Katalin Kamarás
[S-2] November 12, 2013 – University of Nottingham, United Kingdom, Katalin Kamarás
[S-3] June 4, 2014 – University of Geneva, Katalin Kamarás
[S-4] October 2014 – Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland, Gyula Faigel
[S-4] March 11, 2015 – Southwestern University, Georgetown, TX, USA, Katalin Kamarás
[S-5] October 3, 2016 – University of Antwerp, Antwerp, Belgium, Katalin Kamarás
[S-6] March 28, 2017 – Budapest University of Technology and Economics, Katalin Kamarás
[S-7] August 22, 2017 – University of Tennessee, Knoxville, TN, USA, Katalin Kamarás

Outreach:

Popular science articles:

Németh G., Klupp G., Kováts É., Pekker S., Kamarás K.: **Kubán-fullerén kokristályok fázisátalakulásának infravörös spektroszkópiás vizsgálata**
Fizikai Szemle **64,** 310-312 (2014)
Pekker S., Földes D., Kováts É., Bortel G., Jakab E.: **Új szerves-fémkoordinációs vázszerkezetek**
Fizikai Szemle **68,** 11-15 (2018)
Kamarás K.: **Nanotartályok és nanoállványok**
Fizikai Szemle **68,** 8-10 (2018)

Scientific results featured in the popular press:

A-12. *Science Advances* **1,** e1500059-1-9 (2015): Focus (Germany), Physics News
A-21. *Small Methods* **1,** 1700184-1-9 (2017): Index Hungarian news portal