Progress Report – RISE CoExAN (GA644076)

1. General Progress of the action

1.1 Please indicate the progress of the action during the period covered by this report:

- X The action has fully achieved its objectives for the period.
- The action has achieved most of its objectives for the period with relatively minor deviations.
- The action has achieved some of its objectives but corrective action is required.
- The action has failed to achieve critical objectives and/or is severely delayed.

1.2 Please describe the general scientific progress of the action during the period covered by this report (including by giving qualitative indicators and by describing deliverables and milestones achieved):

Free text (maximum 10000 characters)

Overview
More than 70 man-month visits between project partners have been executed during the first 17 months of the project. This has permitted work to start on the principal objectives programmed for this period.
43 articles, 8 of which involve cross-participation of the node partners in the frameworks of the Project, were published in high-impact international journals.
Disseminated results were delivered at 38 prestigious international conferences as invited talks (6 joint).
Participants organized 2 CoExAN special sessions inside Workshops hold in Erice (July 2016) and in Marino at the MIFP workshop (March 2017)

TRANSFER OF KNOWLEDGE:

Qualitative Indicators:

A) CoExAN Publications: 43.

Our scientific outcome was good; in this first year, we published 43 articles related to CoExAN themes, in a variety of international journals. As a direct result of staff exchange, 8 papers have been generated due to newly established collaborations within CoExAN. More joint publications (7) are in preparation and will be soon submitted.

B) Invited Talks in international conferences: 38

C) Conference contributed talks: 13

D) Poster Presentations: 5

E) Scientific Highlight:

Among several excellent articles published within CoExAN, it is worth to highlight the following articles:

A. Mosca Conte, O. Pulci, and F. Bechstedt, "Electronic and optical properties of topological semimetal Cd3As2 from first principles", Scientific Reports (2017) (WP1). Here the authors study a 3D Dirac material, Cd3As2, that is shown to be a 3D analogous to graphene with massless fermions near the Fermi energy.

A. A. Varlamov, A. V. Kavokin, and Y. M. Galperin, "Quantization of entropy in a quasi-two-dimensional electron gas", Physical Review B 93, 155404 (2016) where the authors show that the Entropy in a 2-dimensional system is quantized and its quantum value is universal (WP2)

Another noteworthy article is by, M. De Crescenzi, I. Berbezier, M. Scarselli, P. Castrucci, M. Abbarchi, A. Ronda, F. Jardali, J. Park, and H. Vach, "Formation of Silicene Nanosheets on Graphite" ACS Nano, 10 (2016). The authors confirmed the metallic character of the deposited silicene and show that their samples have excellent agreement with their band structure calculations which exhibit the presence of a Dirac cone. (WP3)

TRAINING:

F) Inter-node Seminars:

Seconded researchers are fully included in the research activities of the host node, are given training, and are also requested to give seminars. Seminars can be formal, for the full host Department, or more informal, lesson-like, often organized on a daily-basis. These have been shown to be extremely useful in training the early stage researchers in the host institution.

While we can quantify the number of inter-node formal seminars given in the hosts institutions by the guests researchers (16), the number of informal seminars can only be estimated (above 50).

G) Dissemination

- Special Dissemination Session in the Physical-mathematical lyceum "Quantum" of the Yerevan University, May, 20, 2016:
  -A. Varlamov Superconductivity: 100 years of discoveries, hopes and delusions.
  -A. Kavokin, Liquid light.
- January 30, 2017 on the TV channel ONT broadcast (Belarus) a new issue of the talk show "The Case of Principle", dedicated to the Belarusian science in ERA.As a guest, INP BSU team member *Prof. Sergey Maksimenko*, was invited
  The program is available at: https://www.youtube.com/watch?list=PLuGCnujoOtrcYZz3b3CVGDJsIkmajrAe&v=GD1P7fIdTf4
- *Prof. Maurizia Palummo* at the Scientific Lyceum "Cartesio", Olevano Romano, Italy 10.03.2017 Dissemination on material science with main focus on nanomaterials, their fashinating properties and applications
- 3 newspaper interviews of *Prof. Maksimenko, Dr. Kuzhir, Dr. Batrakov* concerning their participation in EU research project COEXAN
- *Yuri Svirko and Sergey Maksimenko* guest Editors of Special Issue in „Carbon nanooptics" in Journ. Of Nanophotonics our participation in EU research project COEXAN
- Article on CoExAN in the journal 'Platinum' dedicated to R&D in Italy (Issue November 2016)

H) Awards:

- **Alesia Paddubskaya**, researcher at INP BSU**:** ***1st prize for the best poster*** "Terahertz properties of graphene/polymer sandwich structures" (out of more than 110) in the FM@NT conference, October 5th - 8th, 2015, Vilnius, Lithuania Alesia Paddubskaya, researcher at INP BSU
- **Alesia Paddubskaya**, researcher at INP BSU**:** ***Prize of IAAM Young Scientist Medal - 2016 at Global Graphene Forum*** for the Poster "Excellent microwave absorption in Graphene/polymer sandwiches".
- **Andrey Varlamov,** research director of CNR: ***Grand Prix Public Roberval 2015*** (for the best francophone scientific popular text) "Le Kaleidoscope de la Physique".
- **Davide Grassano,** PhD student at URTV, got the best poster award at the Workshop 'Ugo Fano prize' (19-21 December, CNR, Rome, Italy)

I) Impact: Skills acquisitions:

The seconded staff members (especially the ESRs) are trained in writing papers, writing small projects (for example HPC supercomputer time to perform ab-initio calculations) and more confidence in giving presentations is gained thanks to the large number of presentations by the seconded staff.

J) *Impact: Career Development*:

Roman Polozkov (UI) and Maurizia Palummo (URTV) upgraded to professorship; 2 ESR in BSU upgraded to Researchers; one ESR from UI upgraded to Researcher.

NETWORKING:

K) *Secondments* : 23 researchers have been seconded during the first 17 months of CoExAN, for a total of 53 inter-nodes travels, corresponding to more than 70 man-months

L) Workshops/conferences/special sessions devoted to CoExAN:

- ***ERICE COEXAN JULY 2016:***

  School at the Ettore Majorana Center and special session on "Collective Excitations in Advanced Nanostructures (CoExAN)" (26 July 2016 Erice) within EPIOPTICS-14/Silicene-2 school http://www.ism.cnr.it/it/workshop/epioptics-14/

- Session dedicated to CoExAN at the Mediterranean Institute of Fundamental Physics March meeting (MIFP, www.mifp.eu)

Exploitation:

The immediate targets of CoExAN are fundamental. However, we expect the fundamental results to lead to potential future applications. Possible patents of new synthesis techniques which could be used by UEF startups as end-users are under consideration.

Progresses towards Deliverables and Milestones:

The deliverables due before or at the 17th month were all satisfactory reached, and we are actively working on the future deliverables. Below a summary:

D1.1 Report on electronic density of states by ab-initio methods in carbon nanostructures of increasing sizes.

In progress. Carbon Nanoribbons of increasing size have been considered, together with a BN/C nanoribbons. The density of states and electronic band structure has been calculated at the DFT level, and the gap estimated (URTV). The possibility to grow silicene on graphite is under theoretical consideration (ISP).

D1.2 Report on optical spectra by ab-initio methods in carbon nanostructures of increasing sizes

In progress. The optical properties of silicene have been calculated at the DFT+GW+BSE level. Excitonic effects are shown to be important but a cancellation of Many-body effects is found. The optical properties of C nanoribbons has been calculated at the independent particle level (DFT-RPA).

D1.3. Energy band structure of shaped bilayered graphene nanoribbons.

In progress. The energy band structure was calculated using tight-binding method (UNEXE). The electronic properties of graphene bilayer and nanoribbons has been calculated within Density Functional Theory (URTV). The study of many-body effects is still work in progress. The following problems were investigated:

1. edge states in shaped graphene nano-ribbons;
2. conductor/dielectric transmission depending on nanoribbon boundary shape;
3. tuning of band-gap by external electric field
4. strain effects on graphene

D2.1. Theoretical results for plasmon polariton modes and their instability increments in graphene structures in the presence of electron flows *Completed.*

D2.2. Theory of induced EM generation in graphene structures in the presence of acoustic wave. In progress.

Dispersion equations corresponding to linearized self-consistent equations for system “electron beam + electromagnetic wave” in graphene structures were investigated. The following parameters were estimated

1. Instability increments;

2. Wavelength tuning by variation acoustic wave frequency and propagation direction.

D2.3. Theoretical estimates of induced EM generation parameters in graphene vs applied external bias. Theoretical study of interband THz transitions and excitonic effects in quasi-metallic CNTs and CNT arrays (Task 2.7).

Tight-binding calculations of optical transitions probabilities in electrically biased bilayer graphene clusters have been performed, results reported and published. The study of optical gain in biased structures is still work in progress.

1. Selection rules for optical transitions in quasi-metallic carbon nanotubes with small curvature-induced energy band gaps have been derived.
2. Quasi-exact solutions to the quantum relativistic two-body problem were obtained for a variety of one-dimensional potentials.
3. The excitonic states in narrow-gap single-walled carbon nanotubes have been calculated, the eigenvalues expressed as a function of effective potential width and depth, and the wave functions at zero separation have been determined.
4. In progress: Calculations of the absorption coefficient via the Elliot formula using the two-body wave functions at zero separation.

D3.1. The series of experimental samples of graphene/polymer sandwiches. Completed.

D3.2. Experimental samples of GNRs, mono- and a few layered graphene

In progress. Samples of the mono- and a few layered graphene on metal and dielectric substrates have been delivered.

D3.4. Reports on the structural characterization of experimental samples produced within Tasks 3.1-3.2 .

The properties of the fabricated samples have been reported.

D4.1. Experimental report on the EM response properties of all the produced samples within WP3 in microwave range.

In progress. Microwave measurements of :

1. pyrolytic carbon (PyC) films sandwiched between PMMA (produced by UEF)
2. composite consisting of graphene and PyC (produced by UEF)
3. multilayred graphene (multiGr) sandwiched between PMMA (produced by UEF)
4. self suspending CNT-sponges of different density (produced by ToV)
5. self-supported CNT films made of single, double and multi-walled CNTs (produced by INP BSU)
6. Pyrolyzed photoresist (thicknes 30 nm) (produced by UEF)

D4.2. Experimental report on the THz transmission properties of graphene and nanocarbon based samples, including in some cases temperature dependencies of THz transmission.

In progress. A time-domain terahertz spectrometer (EKSPLA, Vilnius Lithuania) based on femtosecond laser (wavelength 1 µm, pulse duration less than 150 fs) and GaBiAs photoconductive switch as THz emitter and detector was used from 100 GHz to 3 THz for measurements of transmission and in some cases absorption of the following samples

1. PyC films on the top of quartz substrate (produced by UEF)
2. 1-3 graphene layers separated by 100 nm thick PMMA film, free standing (produced by UEF)
3. self-supported CNT films made of single-walled, double-walled and multi-walled CNTs (produced by INP BSU).

D4.3. The data base of high frequency material parameters (dielectric permittivity and conductivity) of graphene and carbon nanostructures in THz and sub-THz ranges.

In progress. Whenever possible material parameters (ac conductivity, dielectric permittivity) were reconstructed from the data measured within the implementation of WP4 (INP BSU)

D4.4. The recommendations to the executors of WP3 "Synthesis".

In progress. Computational modeling with CST studio of electromagnetic response properties of graphene, other thin carbon films and heterostructures as well as CNT arrays and sponges have been done for estimations of the best candidate for being used as the basic material for possible generation of THz radiation experimental observations. (INP BSU).

D5.1 Composition of the task force and kickoff meeting.

Completed. The kickoff meeting was held on the 12th November 2015 by skype. All PIs were present. The task force board was selected.

D5.2 List of work progress indicators; design of the Web site and development of interactive communication tools. Status: 100%

Completed . The list of performance indicators was selected. The webpage has been organized (http://coexan .roma2.infn.it and http://inp.bsu.by/coexan/index.html)

D5.3 Progress meetings. Status: 50%

We have planned 4 progress meetings in the 4 years, two have taken place.

-The 1st progress meeting was held in Minsk at the INP-BSU node, in June 2016.
-The second was held in Rome (20th March 2017) on occasion of the Mid Term Meeting.
-The 3rd will be in Armenia, organized by the YSU node, in 2018.
-The 4th will probably take place in Minsk (INP-BSU node) in June 2019.

Regular meetings between tasks and deliverables responsible scientists take place via Skype.

D5.4 Two Summer schools for ESRs. Status:50%

In progress. We have already held the first school: EPIOPTICS school at the Ettore Majorana Center (Erice, Italy) July 2016. The second will be organized by the UEF in 2018 in Finland (Nanophotonic school).

D5.5 Special sessions on international conferences: in progress. We have organized CoExAN sessions at the MIFP meeting (Marino, Italy, March 2017) and we are organizing a session at the TERAMETANANO conference (Venice, May 2017)

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2. Corrective Measures

2.1 Please explain any delays accumulated in the secondments / activities / deliverables foreseen in the Grant Agreement and the measures taken to oversee them.*Free text (maximum 10000 characters)*

We do not have any delay in the scientific activity.
We had to face two major problems in this 1st year. The first one was related to the delay in the acceptance of the Amendment. It took more than 6 months to include CNR as a new node. This meant that the CNR researchers could not travel for 6 months. We have solved this problem reshuffling some secondments and redistributing some tasks.

The second problem we had to face was related to the sad news that Prof. Gagik Kryuchkyan , PI of the Armenian node, passed away after several months of sickness. His group managed to carry on the scientific tasks, and a new PI has by now been selected, Prof. Hayk Sarkisyan.

The 3 underspending nodes are UEF, URTV, YSU. UEF and URTV accumulated delays in secondments because of an (unforeseen) lack of ESRs. They have solved the problem by hiring new PhD students, who will be eligible for traveling after 6 months from when their employment has started. YSU has accumulated delays because of the sad departure of the YSU Principal Investigator. With the appointment of the new PI, things are now normalizing.

On the other hand, some nodes (UI, CNR, DLSU) are overspending. This makes the percentage of accomplished secondments, as compared to the promised ones, as high as 83%.

2.2 Please indicate any potential risks identified and suggested approaches to mitigate them.

Free text (maximum 5000 characters)

The major risks at this stage come from the technological limitations of the quality of available samples.
The quality of the GNR fabricated via postprocessing of continuous graphene sheets do not always meets requirements. An alternative route, which relies on the direct deposition of graphene/PyC nanoribbons using sacrificial copper films, has been proposed.
Moreover, we mitigate this risk collaborating with several laboratories across Europe, in China and Japan who produce record quality samples of graphene/BN sturctures and transition metal dichalcogenides. We provide regular feedback to the growers which allows them to optimise the growth protocol and improve the quality of the samples.

3. Ethical Issues

Please indicate how the ethical issues have been addressed during the period covered by this report and mention all the approvals/authorisations already provided to the REA (if applicable).

Free text (maximum 5000 characters)

No Ethical issue

4. Additional information

Please indicate any additional information which you may consider useful to assess the project implementation during the period covered by this report, including management issues.

Free text (maximum 5000 characters)

The overall management of the project is done on the day-to-day basis by virtue of the on-line telecommunication between the Scientists in Charge.

The monitoring of milestone achievements is periodically done by skype management meetings.

We have signed a Partnership Agreement among all nodes.

We have established a Decision-Making structure: a Task Force team has been selected at the kickoff meeting (D5.1)

APPENDIX

PUBLICATIONS (Total - 43)

1. V. Shahnazaryan, I. A. Shelykh and O. Kyriienko, Attractive Coulomb interaction of 2D Rydberg excitons, PHYSICAL REVIEW B, 93, 245302 (2016) **WP2**
2. Multiphoton resonant manipulation of qubits by train of pulses, Gor A. Abovyan and Gagik Yu. Kryuchkyan, Opt. Soc. Am. B 33, 971-979 (2016) **WP2**
3. Selective excitations of a Kerr-nonlinear resonator: exactly solvable approach, A.Shahinyan, A. Tamazyan, G. Kryuchkyan, Eur. Phys. J. D (2016) 70: 131. **WP2**
4. Phase locking and quantum statistics in a parametrically driven nonlinear resonator, G. H. Hovsepyan, A. R. Shahinyan, Lock Yue Chew, and G. Yu. Kryuchkyan, Phys. Rev. A 93, 043856, 2016 **WP2**

5. Quantum statistics in a time-modulated exciton-photon system, G. Yu. Kryuchkyan, A. R. Shahinyan, and I. A. Shelykh Phys. Rev. A 93, 043857, 2016 **WP2**
6. L. H. Guessi, Y. Marques, R. S. Machado, K. Kristinsson, L. S. Ricco, I. A. Shelykh, M. S. Figueira, M. de Souza, and A. C. Seridonio, **Quantum phase transition triggering magnetic BICs in grapheme, Phys. Rev. B 92, 245107 (2015) WP1 WP2**
7. C.A.Downing and M.E.Portnoi, Magnetic quantum dots and rings in two dimensions. *Phys. Rev. B* **94**, 045430 (2016). http://dx.doi.org/10.1103/PhysRevB.94.045430 **WP2.**
8. H.Abdelsalam, M.H.Talaat, I.Lukyanchuk, M.E.Portnoi, and V.A.Saroka, Electro-absorption of silicene and bilayer graphene quantum dots. *J. Appl. Phys.* **120**, 014304 (2016). http://dx.doi.org/10.1063/1.4955222 **WP1 WP2**
9. V.A. Saroka and K.G. Batrakov, Zigzag-Shaped Superlattices on the Basis of Graphene Nanoribbons: Structure and Electronic Properties. *Russian Physics Journal* **59**, 27–32 (2016). http://doi.org/10.1007/s11182-016-0816-6 (Joint publication with INP BSU) **WP1 WP2**
10. A.M.Alexeev, R.R.Hartmann, and M.E.Portnoi, Two-phonon scattering in graphene in the quantum Hall regime. *Phys. Rev. B* **92**, 195431 (2015). http://dx.doi.org/10.1103/PhysRevB.92.195431 **(WP2)**
11. R.R. Hartmann and M.E. Portnoi /Exciton states in narrow-gap carbon nanotubes // Proceedings of the 1st Conference on Progress in Applied Mathematics in Science and Engineering, Bali Indonesia, October 2015 / AIP Conference Proceedings **1705**, 020046 (2016). (Joint work with DLSU) **WP2**
12. V.A. Saroka, R.R. Hartman and M.E. Portnoi / Terahertz transitions in narrow-gap carbon nanotubes and graphene nanoribbons // Proceedings of 24th International Symposium Nanostructures: Physics and Technology, St Petersburg, Russia, June 27 – July 1, 2016 / Editor: E. Kholmogorova. — St Petersburg, Academic University Publishing 2016. — P.205–206. ISBN 978-5-7422-5323-5 (Joint work with DLSU) **WP2**
13. T. Kaplas, L. Karvonen, S. Ahmadi, B. Amirsolaimani, S. Mehravar, N. Peyghambarian, K. Kieu, S. Honkanen, H. Lipsanen, and Yuri Svirko, "Optical characterization of directly deposited graphene on a dielectric substrate", *Optics Express* 24, 2965 – 2970 (2016). DOI:10.1364/OE.24.002965**. (WP3, WP4)**
14. Mahesh Kumar, Jani Tervo, Tommi Kaplas, Yuri Svirko "Graphene-enhanced waveguide resonance gratings" *Journal of Nanophotonics* **10**, 012518 (2016). DOI: 10.1117/1.JNP.10.012518 (**WP2**, **WP3**))
15. Galyna I Dovbeshko, Volodymyr R Romanyuk, Denys V Pidgirnyi, Vsevolod V Cherepanov, Eugene O Andreev, Vadim M Levin, Polina P Kuzhir, Tommi Kaplas and Yuri P Svirko, "Optical properties of pyrolytic carbon films versus graphite and graphene", *Nanoscale Research Letters* 10, 163 (2015); DOI 10.1186/s11671-015-0946-8 **WP3, WP4**
16. *Temperature-dependent excitonic effects in the optical properties of single-layer MoS 2*, A Molina-Sánchez, M Palummo, A Marini, L Wirtz
Physical Review B 93 (15), 155435 (2016) **WP1**
17. *Crystal phase effects in Si nanowire polytypes and their homojunctions*, M Amato, T Kaewmaraya, A Zobelli, M Palummo, R Rurali will appear in: Nano Letters 2016 10.1021/acs.nanolett.6b02362 **WP1**
18. Optical and Electronic Properties of Two-Dimensional Layered Materials
M Bernardi, C Ataca, M Palummo, JC Grossman, Nanophotonics 5,111 (2016) DOI 10.1515/nanoph-2015-0030 **WP1**

19. "Ultrafast dynamics in unaligned MWCNTs decoratedwith metal nanoparticles", G. Manzoni, S. Ponzoni, G. Galimberti, M. Scarselli, O. Pulci, L. Camilli, L.Matthes, P. Castrucci, and S. Pagliara, Nanotechnology 27, 235704 (2016) (**WP1**, **WP3**)

20. K. G. Batrakov, A. G. Paddubskaya, N. I. Valynets, S. P. Voronovich-Solonevich, P. P. Kuzhir, S. A. Maksimenko, T. Kaplas, and Yu. Svirko, MICROWAVE ABSORPTION IN GRAPHENE FILMS: THEORY AND EXPERIMENT, Journal of Applied Spectroscopy, Vol. 83, No. 4, September, 2016 (Russian Original Vol. 83, No. 4, July–August, 2016) DOI 10.1007/s10812-016-0342-x **WP2, WP3 and WP4**).

21. A. A. Varlamov, A. V. Kavokin, and Y. M. Galperin, ***Quantization of entropy in a quasi-two-dimensional electron gas*.** PHYSICAL REVIEW **B 93**, 155404 (2016) **WP1**

22. A. Pourret, S.G. Sharapov, A.A. Varlamov, and Gertrud Zwicknagl, ***Cascade Lifshitz transitions in $YbRh_2S_2$ under the effect of magnetic field and related anomalies in Seebeck coefficient***, *submitted to* PHYSICAL REVIEW, September, 2016. **WP2**

23. L. Matthes, O. Pulci, F. Bechstedt, *Influence of out-of-plane response on optical properties of two-dimensional materials: First principles approach (submitted)* **WP1**

24. PolinaKuzhir, AlesiaPadabskaya, NadezhdaVolynets, Konstantin Batrakov, Tommi Kaplas, PatriziaLamberti, RumianaKotsilkova, Philippe Lambin, *The main principles of passive devices based on graphene and carbon films in microwave - THz frequency range*, J. Nanophoton. 11(3), 032504 (2017), doi: 10.1117/1.JNP.11.032504 (**WP4**)

25. C. A. Downing, M. G. Robinson, M. E. Portnoi "Nanohelices as superlattices: Bloch oscillations and electric dipole transitions", Physical Review B 155306-1 - 155306-6 (2016) 95 10.1103/PhysRevB.94.155306 **(WP2)**

26. Maria Stella Prete, Adriano Mosca Conte, Paola Gori, Friedhelm Bechstedt, Olivia Pulci
" Tunable electronic properties of two-dimensional nitrides for light harvesting heterostructures" Applied Physics Letters 110, 012103 (2017) 10.1063/1.4973753 **(WP1)**

27. Yafeng Wang, Liming Liao, Tao Hu, Song Luo, Lin Wu, Jun Wang, Zhe Zhang, Wei Xie, Liaoxin Sun, A. V. Kavokin, Xuechu Shen, and Zhanghai Chen," Exciton-Polariton Fano Resonance Driven by Second Harmonic Generation", Physical Review Letters 118 063602 (2017) 10.1103/PhysRevLett.118.063602 (WP2)

28. A. Mosca Conte, O. Pulci, and F. Bechstedt "Electronic and optical properties of topological semimetal Cd3As2 from first principles", Scientific Reports 2017 DOI:10.1038/srep45500 **(WP1)**

29. Junji Jia, P. K. Pyatkovskiy, E. V. Gorbar, and V. P. Gusynin "Broken symmetry states in bilayer graphene in electric and in-plane magnetic fields", Physical Review B 045410 95 (2017) 10.1103/PhysRevB.95.045410 (WP2)

30. "Nonequilibrium Anderson Model Made Simple with Density Functional Theory", Stefan Kurth and Gianluca Stefanucci Physical Review B 94, 241103(R) (2016). https://doi.org/10.1103/PhysRevB.94.241103 **(WP1)**

31. V. P. Gusynin and P. K. Pyatkovskiy Critical number of fermions in three-dimensional QED Physical Review D94/12 125009 2470-0010 (2016) 10.1103/PhysRevD.94.125009 **(WP2)**

32. Enrico Perfetto, Davide Sangalli, Andrea Marini and Gianluca Stefanucci, "First-Principles Approach to Excitons in Time-Resolved and Angle-Resolved Photoemission Spectra", Physical Review B 94, 245303 (2016) https://doi.org/10.1103/PhysRevB.94.245303 **(WP1)**

33. Yaroslav Pavlyukh, Anna-Maija Uimonen, Gianluca Stefanucci and Robert van Leeuwen, "Vertex Corrections for Positive-Definite Spectral functions of Simple Metals", Physical Review Letters 117, 206402 (2016) https://doi.org/10.1103/PhysRevLett.117.206402 (WP1,WP2)

34. Yang Kaike, Enrico Perfetto, Stefan Kurth, Gianluca Stefanucci and Roberto D'Agosta Density Functional Theory of the Seebeck Coefficient in the Coulomb Blockade Regime", Physical Review B 94, 081410(R) (2016) https://doi.org/10.1103/PhysRevB.94.081410 **WP1,WP2**

35. E. Baldini, L. Chiodo, A. Dominguez, M. Palummo, S. Moser, M. Yazdi-Rizi, G. Auböck, B.P.P. Mallett, H. Berger, A. Magrez, C. Bernhard, M. Grioni, A. Rubio, M. Chergui. Strongly bound excitons in anatase TiO2 single crystals and nanoparticles. To appear on Nature Communications 2017 WP1

36. O. V. Kibis, K. Dini, I. V. Iorsh, and I. A. Shelykh All-optical band engineering of gapped Dirac materials PHYSICAL REVIEW B 1098-0121 2017 https://doi.org/10.1103/PhysRevB.95.125401 **WP2**

37. G. Yu. Kryuchkyan, V. Shahnazaryan, O. V. Kibis, and I. A. Shelykh Resonance fluorescence from an asymmetric quantum dot dressed by a bichromatic electromagnetic field PHYSICAL REVIEW A 1094 (2017) https://doi.org/10.1103/PhysRevA.95.013834 **WP2**

38. Y. Marques, L. S. Ricco, F. A. Dessotti, R. S. Machado, I. A. Shelykh, M. de Souza, and A. C. Seridonio Realization of anomalous multiferroicity in free-standing graphene with magnetic adatoms PHYSICAL REVIEW B 1098 (2016) https://doi.org/10.1103/PhysRevB.94.205119 **WP2**

39. Ivan I. Vrubel, Roman G. Polozkov , Ivan A. Shelykh, Vasilii M. Khanin, Piotr A. Rodny, and Cees R. Ronda Bandgap Engineering in Yttrium–Aluminum Garnet with Ga Doping Crystal Growth & Design 1528 (2017) 10.1021/acs.cgd.6b01822 **WP2**

40. Maurizio De Crescenzi, Isabelle Berbezier, Manuela Scarselli, Paola Castrucci, Marco Abbarchi, Antoine Ronda, Fatme Jardali, Jejune Park, and Holger Vach. Formation of Silicene Nanosheets on Graphite ACS Nano, 10 (2016), 11163−11171 DOI: http://dx.doi.org/10.1021/acsnano.6b06198 **WP3**

41. Francesco De Nicola, Matteo Salvato, Carla Cirillo, Michele Crivellari, Maurizio Boscardin, Manuela Scarselli, Francesca Nanni, Ilaria Cacciotti, Maurizio De Crescenzi, Paola Castrucci Record efficiency of air-stable multi-walled carbon nanotube/silicon solar cells, Carbon 101 (2016) 226-234 http://dx.doi.org/10.1016/j.carbon.2016.01.099 **WP3**

42. F. Rigoni, C. Pintossi, G. Drera, S. Pagliara, G. Lanti, P. Castrucci, M. De Crescenzi & L. Sangaletti A cross-functional nanostructure platform based on carbon nanotube-Si hybrid junctions: where photon harvesting meets gas sensing; Scientific Reports 7 (2017) 44413 http://dx.doi.org/10.1038/srep44413 **WP3**

43. Kuzhir P., Paddubskaya A., Volynets N., Batrakov K., Maksimenko S. , E. Golubeva, Valusis G., Kaplas T., N.Reckinger, Lobet M. , Lambin Ph., Graphene/polymer multilayers at high frequencies: no effect of graphene grain size on the electromagnetic shielding effectiveness, accepted Journal of Nanophotonics, 2017 **WP3**

INVITED PRESENTATIONS AT CONFERENCES (Total -38)

1. O. Pulci IW2DC International workshop (Campofelice di Roccella, 29, May-4 June (2016) WP1
2. O. Pulci Invited talks (2 classes) at the EPIOPTICS 2016 school (Erice, 24-30 July 2016) WP1
3. M. Palummo "Fundamental properties of transition metal dichalcogenides: novel 2d materials for opto-electronic applications" NN2016, Frascati, September, 27, 2016 WP1
4. M. Palummo "Transition Metal Dichalcgenides: 2D materials for next generation opto-electronic devices" Fall Meeting EMRS 2016 September, 18-22, 2016 WP1
5. O. Pulci, "Ab-initio study of new materials: from 2D Nitrides to 3D Dirac systems" (seminar) 31 Friedrich Schiller Universitaet Jena, August, 2016 WP1
6. M. Palummo 'Light absorption and exciton radiative lifetimes in two-dimensional transition metal dichalcogenides', Nanoscience and Nanotechnology, INFN, Frascati, October, 1, 2015 WP1
7. M. Palummo "Transition metal dichalcogenides: a novel class of two-dimensional materials for opto-electronics', ICN2, Istitut Catala' de Nanocienca i Nanotecnlogia, Barcelona 21/1/2016 WP1
8. M.E.Portnoi. "Terahertz Transitions in Narrow-Gap Carbon Nanotubes and Graphene Nanoribbons" Energy Materials and Nanotechnology (EMN) Meeting, Hong Kong. 9-12/12/2015 – / http://www.emnmeeting.org/hongkong/terahertz-technology/ (WP2)
9. M.E.Portnoi 28-31/03/2016 – 17th International Conference on Physics of Light-Matter Coupling in Nanostructures (PLMCN17), Nara, Japan. Talk "Zero-energy vortices in graphene " / M.E. Portnoi. http://www.plmcn17.iis.u-tokyo.ac.jp/invited.html (WP2)
10. M.E.Portnoi 29/05-04/06/2016 – International Workshop on Physics of 2D Crystals, Campofelice di Roccella, Sicily. Talk "Zero-energy vortices in two-dimensional Weyl semimetals" / M.E.Portnoi. http://www.mifp.eu/SCHOOLS/IW2DC-2016/workshop-program.html (WP2)
11. M.E.Portnoi 27/06-02/07/2016 – International Summer School and Workshop "Nanostructures for Photonics", NSP 2016, St Petersburg, Russia. Talk "Carbon-based nanostructures for THz applications" / M.E.Portnoi. http://lpc.ifmo.ru/nsp2016/page/64/Speakers.htm (WP2)
12. Ivan A. Shelykh1 , Skender Morina , Kristinn Kristinsson , Kevin Dini, Oleg Kibis, Transport properties of electromagnetically dressed grapheme, META'16(2016) WP1,3
13. D. Gulevich, A. P. Alodjants, I. A. Shelykh, Tunable Josephson Effect in Exciton Polariton Bose Einstein Condensates, PMLCN17, (2016) WP2

14. I. Shelykh, H. Sigurdsson and O. V. Kibis, Analogue of Aharonov-Bohm phase induced by circular polarized light in mesoscopic quantum rings and metamaterial, PMLCN17,(2016) WP2
15. T. Espinosa-Ortega, T. C. H. Liew, I. A. Shelykh, Polaritonics: Optical Diodes and Neural Networks, PMLCN17,(2016) WP2
16. H. Sigurdsson , I. A. Shelykh, T. C. H. Liew, Switching Waves in Multi Level Incoherently Driven Polariton Condensates, PMLCN17,(2016) WP2
17. D.Yudin, O.V.Kibis, I.A. Shelykh, Optical Control of Spin Charge Dynamics in Topological Insulators PMLCN17,(2016) WP2
18. I.A. Shelykh "Transport and spin properties of graphene and topological insulators in the regime of electromagnetic dressing", The Sixth Annual Meeting of the members of the Mediterranean Institute of Fundamental Physics(2016) WP3
19. S. Morina, O. V. Kibis, A. A. Pervishko, I. A. Shelykh, Transport and Spin Properties of 2DEG Dressed by Light, SIM (2016) WP2
20. H. Sigurdsson, O. E. Egorov, X. Ma, I. A. Shelykh, T. C. H. Liew, Information processing with topologically protected vortex, memories in exciton-polariton condensates , OECS-2015 (2015) WP2
21. S. Morina, A. A. Pervishko, K. Kristinsson, O.V.Kibis, I.A. Shelykh, Control of the transport properties of two-dimensional systems by a high-frequency dressing field, IMMEA-2015(2015) WP2
22. V. Shahnazaryan, O. Kyriienko , I. A. Shelykh, Adiabatic preparation of a cold exciton condensate, IMMEA-2015(2015) WP1
23. Photon blockade via frequency-chirped excitations G. H. Hovsepyan , V. A. Manukyan and G. Yu. Kryuchkyan, LPHYS 2016 WP2
24. Spatio-spectral characteristics of biphotons in structured nonlinear waveguides A. Tamazyan, G. Kryuchkyan, LPHYS 2016 WP2
25. Nonclassical States in Spatially Overlapping Semiconductor Cavities
    G. Yu. Kryuchkyan, A R Shahinyan, I. A. Shelykh, LPHYS 2016 WP2
26. Resonance Fluorescence in Double Driven Asymmetric Quantum Dot
    G Y Kryuchkyan , O V Kibis , V A Shahnazaryan, I A Shelykh, LPHYS 2016 WP2
27. Yu. P. Svirko, Sythesis of graphen and ultrathin pyrolytic carbon films on dielectrics. School for Young Researchers "Carbon nanotubes and graphene; new horizons", Moscow, Prokhorov Institute of general Physics, December 1-4, 2015 (wp 3)
28. Polina Kuzhir, Konstantin Batrakov, Sergey Maksimenko, Philippe Lambin, Tommi Kaplas, Yuri Svirko, Absorption of electromangtic radiation in ultra-thin graphene films: theory and experiment, School for Young Researchers "Carbon nanotubes and graphene; new horizons", Moscow, Prokhorov Institute of general Physics, December 1-4, 2015 (wp2,3 and 4)
29. Tommi Kaplas and Yuri Svirko, Direct Deposition of a Graphitic Film on a Dielectric Substrate by Nickel Nanocatalyst. 5th International Workshop on Nanocarbon Photonics and Optoelectronics (1-6 August 2016, Imatra, Finland) (Wp3)
30. Tommi Kaplas : Graphene and pyrolytic carbon: SynthesisUniversity of California, 11.12.2015, Riverside, California (WP3)
31. Review Lecture: A.A. Varlamov. Electronic topological transitions (Lifshitz transitions of the 2½ order). CEA, Grenoble, organized within CoExAN, February, 15, 2016. WP1
32. Review Lecture: A.A. Varlamov. Fluctuoscopy of Superconductors and Dynamics of Abrikosov's Lattice Formation Close to $H_{c2}(0)$. CEA, Grenoble, organized within CoExAN, February, 22, 2016 WP1.

33. S. A. Maksimenko, K. G. Batrakov, P. P. Kuzhir, M. V. Shuba, G. Y. Slepyan, Electromagnetic effects in nanocarbon: modelling and device applications, XIV International Conference onQuantum Optics and Quantum Information, October 27–30, 2015, Minsk, BELARUS (wp2)
34. Polina Kuzhir, Konstantin Batrakov, Sergey Maksimenko, Philippe Lambin, Tommi Kaplas, Yuri Svirko, Absorption of electromangtic radiation in ultra-thin graphene films: theory and experiment, School for Young Researchers "Carbon nanotubes and graphene; new horizons", Moscow, Prokhorov Institute of general Physics, December 1-4, 2015 (wp2,3 and 4)
35. K. Batrakov, P. Kuzhir, S. Maksimenko, Propagation and generation of THz electromagnetic waves in multi-walled CNTs and multi-layered graphene, EMN Meeting on metamaterials, Dubrovnik, Croatia, May 8 - 12, 2016. http://emnmeeting.org/ metamaterials/
36. K. Batrakov, P. Kuzhir, S. Maksimenko, G. Slepyan, Electromagnetic Effects in Carbon Nanotubes and Multi-Layered Graphene, International School of Solid State Physics EPIOPTICS-14/SILICENE-2, 24 – 30 July 2016 ERICE, SICILY, http://www.ism.cnr.it/en/workshop/epioptics-14/
37. P. Kuzhir, K. Batrakov, S. Maksimenko, A. Paddubskaya, Tommi Kaplas, Yuri Svirko, Philippe Lambin, Graphene based microwave – THz devices: main principles, tutorial lecture (the invited talk) School for Young Researchers "Nanocarbon for Optics and Electronics", Kaliningrad (Russia) 24 - 29 July, 2016,The Emmanuel Kant Baltic Federal University (wp2,3 and 4)
38. Polina Kuzhir, Konstantin Batrakov, Alesia Paddubskaya, Sergey Maksimenko, Rumiana Kotsilkova, Tommi Kaplas, Yuri Svirko, Philippe Lambin, Graphene heterostructures: peculiarities of microwave and THz response, The Fifth International Workshop on Nanocarbon Photonics and Optoelectronics will be held from 1 until 5 August, 2016 at the Holiday Club Saimaa,Imatra, South Karelia, Finland. (wp2,3 and 4)

ORAL PRESENTATIONS (13)

1. M.S. Prete, O. Pulci, "Two Dimensional Nitrides: an initio-study" in March 2016 for the E-Cost Optical Nanospectroscopy III Conference
2. M. Prete, O. Pulci" Two dimensional systems: an ab-initio study" at Nanoscience and Nanotechnology conference INFN-Frascati
3. 27/06-01/07/2016 – Nanostructures: Physics and Technology, St Petersburg, Russia. Talk "Terahertz transitions in narrow-gap carbon nanotubes and graphene nanoribbons", V.A. Saroka, R.R. Hartmann, and M.E. Portnoi. http://www.ioffe.ru/NANO2016/
4. 21-24/09/2016 – International workshop "Novel Terahertz Devices", Prague, Czech Republic. Talk "Terahertz Transitions in Quasi-metallic Graphene Nanoribbons", V. A. Saroka, R. R. Hartmann, and M. E. Portnoi. http://www.notedevworkshop2016.eu
5. R. R. Hartmann and M. E. Portnoi, Electron-hole pairing in narrow-gap carbon nanotubes**,** Advanced Research in Electronic Engineering and Information Technology International Conference, August 23-25 2016
6. **14-18/03/2016** – APS March Meeting 2016, Baltimore, Mariland, USA. Talk "Two-particle vortices in graphene" / M.E. Portnoi and C.A. Downing, Bulletin of the American Phys. Society, **61**(2) https://meetings.aps.org/Meeting/MAR16/Session/K17.5 **(WP2)**

7. **27/06-01/07/2016** – Nanostructures: Physics and Technology, St Petersburg, Russia. Talk "Terahertz transitions in narrow-gap carbon nanotubes and graphene nanoribbons" / V.A. Saroka, R.R. Hartmann, and M.E. Portnoi. http://www.ioffe.ru/NANO2016/ **(WP1, WP2)**
8. **24-30/07/2016** – International School of Solid State Physics, Epioptics-14 and Silicene-2, Erice, Sicily, Italy. Talk "Zero-energy vortices in two-dimensional Weyl materials" / M.E. Portnoi, and C.A. Downing http://www.ism.cnr.it/en/workshop/epioptics-14/ **(WP1, WP2)**
9. **24-30/07/2016** – International School of Solid State Physics, Epioptics-14 and Silicene-2, Erice, Sicily, Italy. Talk "Electro-absorption of silicene and bilayer graphene quantum dots" / V. A. Saroka, H. Abdelsalam, M. H. Talaat, I. Lukyanchuk, M. E. Portnoi, and O. Pulci http://www.ism.cnr.it/en/workshop/epioptics-14/ (Joint work with URTV) **(WP1, WP2)**
10. **21-24/09/2016 –** International Workshop "Novel Terahertz Devices", Prague, Czech Republic. Talk "Terahertz Transitions in Quasi-metallic Graphene Nanoribbons" / V. A. Saroka, R.R. Hartmann, and M.E. Portnoi. http://www.notedevworkshop2016.eu/ (Joint work with DLSU) **(WP2)**
11. P. Kuzhir, K. Batrakov, S. Maksimenko, A. Paddubskaya, G.Valusis, Rumiana Kotsilkova, Tommi Kaplas, Yuri Svirko, Philippe Lambin, Electromagnetic properties of graphene/polymer sandwiches, EMRS Spring meeting, Symposium Y Graphene and related materials: from fundamental science to applications, Lillie France 1-6 may 2016 (wp3 and 4)
12. G. I. Márk, K. Kertész, G. Piszter, I. Biró, P. Kuzhir, Ph. Lambin, and L. P. Biró, 3D printed nanocarbon microwave absorbers, EMRS Spring meeting, Symposium F Advanced materials for printing, Lillie France 1-6 may 2016 (wp3 and 4)
13. A. Plyushch, J. Macutkevic, P. Kuzhir, J. Banys, Dz. Bychanok, S. Maksimenko, A. Cataldo, F.Miciulla, S. Bellucci, Redistribution effects in graphene nano platelets / epoxy resin composite FM&NT-2015 | October 5th - 8th, Vilnius, Lithuania **(wp4)**

POSTER PRESENTATIONS (Total – 5)

1. V.A. Saroka, R.R. Hartmann, and M.E. Portnoi. "Terahertz Transitions in Narrow-Gap Carbon Nanotubes and Graphene Nanoribbons" / (3rd place in Best Poster Award) "Nanostructures for Photonics", NSP 2016, St Petersburg, Russia, **27/06-02/07/2016** – International Summer School and Workshop http://lpc.ifmo.ru/nsp2016// (Joint work with DLSU) (WP2)
2. A. Paddubskaya, K. Batrakov, P. Kuzhir, S. Maksimenko, T. Kaplas, Yu. Svirko, G. Valusis "Terahertz properties of graphene/polymer sandwich structures", FMNT-2015, October 5th - 8th, Vilnius, Lithuania (**wp2 and 4**)
3. P. Kuzhir, K. Batrakov, S. Maksimenko, A. Paddubskaya, G.Valusis, R. Kotsilkova, T. Kaplas, Y. Svirko, P. Lambin, "Excellent microwave absorption in Graphene/polymer sandwiches", Global Graphene Forum, GGF-2016, 23-25 August, 2016, Sweden (**wp2 and 4**)
4. M.S. Prete: "Graphene like two dimensional systems: an ab-initio study" in May 2015 for the gbb60 workshop "Computer simulation for condensed phase systems from correlated electrons to novel material systems.
5. M. S. Prete : "Tunable electronic gap in 2-D: an ab-initio study" in July 2016 for the International School of Solid State Physics, Erice-Sicily