Q@TN - *Quantum Science and Technology in Trento*
APPLICATION FORM
for PhD or postdoctoral fellowship

1. Project title: Quantum sensing with laser-synthesized **NA**no-**DIA**mond NV color centers (NaDia)

2. Keywords: Quantum sensors, nano-diamond synthesis, NV centers, electronic structure simulation, molecular dynamics

3. Type of position requested: PhD student

4. Duration of the position: 36 months

5. Estimated cost of the position: Euro 77,783.83 (cost of a Ph.D. fellowship as of the last deliberation of the University of Trento, Euro 67,780.13, plus 1 year of increment for periods spent abroad, Euro 10,003.69)

6. Managing partner (for PostDocs) / doctoral school (for PhD):

FBK (ECT*)
UniTN (Departments of Physics and Industrial Engineering)
Doctoral School: Physics

7. Proponents (at least two researchers affiliated to different teams)**:**

Simone Taioli (ECT*)

Senior Researcher. Dr. Taioli uses *state-of-the-art* and develops novel theoretical and computational methods for the first principles solution of the many-body problem in nuclei, molecules, and solids. The full CV is attached to this submission.

Recent and on-going projects:

- **ARTIQS:** *"ARTificial Intelligence for Quantum Systems"*(May 2019 - ongoing) **-** postdoctoral call of the Q@TN consortium - total budget 160k €
- **NANOCATH:** *"High-Z ceramic oxide nanosystems for mediated proton cancer therapy"* (December 2019 - ongoing) CARITRO Foundation - total budget 50k €
- **MaDEleNA**: *"Developing and studying novel intelligent nanomaterials and devices towards adaptive electronics and neuroscience applications" (*Dec 2010 - Dec 2015) - Grandi Progetti PAT - total budget 1500k €

- **2SuperB:** *"Epitaxial growth of graphene and SiC layers on inorganic surfaces: a joint theoretical and experimental approach"* (Jan. 2010 - Dec 2010) - FP7 Marie Curie Outgoing Researcher - total budget 30k €

- **MISTICO:** *"New Technologies and Microsystems for solar energy cogeneration solutions"* (March 2011- Feb 2013) - CARITRO Foundation- total budget 120k €

- **NEMESYS**: *"Non equilibrium dynamics models and excited state properties"* (Nov 2016 - ongoing) - INFN strategic project - total budget 300k €

- **SCIENCE FOR PEACE:** "Electron energy loss techniques" in collaboration with Kurchatov Institute (Jan 2011 - Dec 2013) - NATO Collaborative Grant - total budget 20k €

5 publications relevant to the project:

- *A quantum chemical interpretation of two-dimensional electronic spectroscopy of Light-Harvesting complexes,* F. Segatta, L. Cupellini, S. Jurinovich, S. Mukamel, M. Dapor, S. Taioli, M. Garavelli, B. Mennucci, *Journal of the American Chemical Society* 139 (22), 7558 (2017)

- *Tunable band gap in hydrogenated quasi-free-standing graphene,* D. Haberer, D.V. Vyalikh, S. Taioli, B Dora, M Farjam, J Fink, D. Marchenko, T. Pichler, K. Ziegler, S. Simonucci, M.S. Dresselhaus, M. Knupfer, B Buchner, A Gruneis *et al., Nano letters* 10 (9), 3360-3366 (2010)

- *Computational study of graphene growth on copper by first-principles and kinetic Monte Carlo calculations,* S. Taioli, *Journal of molecular modeling* 20 (7), 2260 (2014)

- *Epitaxy of nanocrystalline silicon carbide on Si (111) at room temperature,* R. Verucchi, L. Aversa, M.V. Nardi, S. Taioli, S. a Beccara, D. Alfè, L. Nasi, F. Rossi, G. Salviati, S. Iannotta, *Journal of the American Chemical Society* 134 (42), 17400-17403 (2010)

- *Electron spectroscopies and inelastic processes in nanoclusters and solids: theory and experiment,* Simone Taioli, Stefano Simonucci, Lucia Calliari, Maurizio Dapor, Physics Reports 493 (5), 237-319 (2010)

Antonio Miotello (UniTN)

Full Professor at the Physics department, UniTN, and responsible of IdEA laboratory (Trento University, https://www.physics.unitn.it/en/104/idea-hydrogen-energy-environment).

Research activity on:

- Laser-surface interaction with emphasis on laser absorption, electron excitation, and relaxation.

- Transport and relaxation processes in solids in ordinary conditions and under interaction with fast charged particles.

- Microscopic processes involved in growth of thin films having several composition and structure on different substrates, by using deposition techniques: Physical Vapor Deposition, Ion-Beam Assisted Deposition (IBAD), and Laser-Ablation

- Synthesis of nano-particles of composite materials having catalytic properties in hydrolysis of chemical hydrides

- Synthesis of photocatalysts for water splitting and hydrogen production with photolectrochemical cells.

Recent and ongoing projects:

Generation of electric and thermal energy by means of solar concentrators with parabolic mirrors: study of receivers for Stirling engines and devices for the use of high efficiency solar cells in multi-junction configuration. Fond. CARITRO (2008-2010).

Concentrated thermodynamic solar: production of chemical hydrides rich in hydrogen for direct use in fuel cells with production of electric and thermal energy. Fond. CARITRO (2010-2012).

Project ENAM – Physics, Chemistry, Biotechnology for energy and the environment. Funded by PAT (Autonomous Province of Trento) and CNR (Italian National Research Council) 2014-2018.

ERiCSol - Interdepartmental research area on renewable energy storage and solar fuels (https://projects.unitn.it/ericsol/projects_ericsol/) – Strategic project of the University of Trento.

New Reflections: High Power Laser for ablative propulsion and other space applications INFN 2017-2020.

GLARE-X: Georeferencing via LAser Ranging and LAser debris Redirection from space E-X, INFN 2019-2021.

Five publications relevant to the project:

1) L. Basso, N. Bazzanella, M. Cazzanelli, and **A. Miotello**, On the route towards a facile fluorescent nanodiamonds laser-synthesis, *Carbon* 153, 148-155 (2019).

2) F. Gorrini, R. Giri, C. E. Avalos, S. Tambalo, S. Mannucci, L. Basso, N. Bazzanella, C. Dorigoni**,** M. Cazzanelli, P. Marzola, **A. Miotello**, A. Bifone, Fast and sensitive detection of hemoglobin and

other paramagnetic species using coupled charge and spin dynamics in strongly fluorescent nanodiamonds, *ACS Applied Materials Interfaces* 11, 24412-24422 (2019).

3) L. Basso, F. Gorrini, M. Cazzanelli, N. Bazzanella, A. Bifone, and **A. Miotello**, An all-optical single-step process for production of nanometric-sized fluorescent diamonds, *Nanoscale* 10, 5738-5744 (2018).

4) L. Basso, F. Gorrini, N. Bazzanella, M. Cazzanelli, C. Dorigoni, A. Bifone, **A. Miotello**: The modeling and synthesis of nanodiamonds by laser ablation of graphite and diamond-like carbon il liquid-confined ambient. *Applied Physics A, Materials Science and Processing* 124:72, 7 pages, (2018).

5) F. Gorrini, M. Cazzanelli, N. Bazzanella, R. Edla, M. Gemmi, V. Cappello, J. David, C. Dorigoni, A.Bifone, **A. Miotello**: On the thermodynamic path enabling a room-temperature, laser-assisted graphite to nanodiamond transformation. *Scientific Reports* 6: 35244, (2016).

Michele Orlandi (UniTN)

Assistant professor (RTDB) at the Physics department, UniTN. Active in the application-oriented design and fabrication of materials, combining physical-vapour deposition methods (laser ablation/deposition, RF-magnetron sputtering, e-gun and Joule-effect evaporation) with wet-chemistry synthesis and/or post-processing. The complete CV is attached.

Recent and ongoing projects:

- ERiCSol - Interdepartmental research area on renewable energy storage and solar fuels (https://projects.unitn.it/ericsol/projects_ericsol/) – Strategic project of the University of Trento.

- Project ENAM – Physics, Chemistry, Biotechnology for energy and the environment. Funded by PAT (Autonomous Province of Trento) and CNR (italian National Research Council).

- HiPerDART - Development of High Performance Diagnostic Array Replication Technology (EU-FP7 seventh framework program, Grant agreement ID: 223378), http://hiperdart.eu/ - https://cordis.europa.eu/project/rcn/88961/factsheet/en.

Five publications relevant to the project:

1. Orlandi, M.,* Berardi, S., Mazzi, A., Caramori, S., Boaretto, R., Nart, F., Bignozzi, C.A., Bazzanella, N., Patel, N., Miotello, A. Rational Design Combining Morphology and Charge-Dynamic for Hematite/Nickel-Iron Oxide Thin-Layer Photoanodes: Insights into the Role of the Absorber/Catalyst Junction **(2019)** ACS Applied Materials and Interfaces, 11 , pp. 48002-48012. DOI: 10.1021/acsami.9b19790.

2. Popat, Y., **Orlandi, M.,** Patel, N., Edla, R., Bazzanella, N., Gupta, S., Yadav, M., Pillai, S., Patel, M., Miotello, A. Pulsed laser deposition of CoFe2O4/CoO hierarchical-type nanostructured heterojuction forming a Z-scheme for efficient spatial separation of photoinduced electron-hole pairs and highly active surface area (**2019**) Applied Surface Science, 489, pp. 584-594. DOI: 10.1016/j.apsusc.2019.05.314.

3. Mazzi, A., **Orlandi, M.,** Patel, N., Miotello, A. Laser-inducing extreme thermodynamic conditions in condensed matter to produce nanomaterials for catalysis and the photocatalysis (**2018**) Springer Series in Materials Science, 274, pp. 89-106. DOI: 10.1007/978-3-319-96845-2_4.

4. Edla, R., Tonezzer, A., **Orlandi, M.,** Patel, N., Fernandes, R., Bazzanella, N., Date, K., Kothari, D.C., Miotello, A. 3D hierarchical nanostructures of iron oxides coatings prepared by pulsed laser deposition for photocatalytic water purification (**2017**) Applied Catalysis B: Environmental, 219, pp. 401-411. DOI: 10.1016/j.apcatb.2017.07.063.

5. Orlandi, M.,* Caramori, S., Ronconi, F., Bignozzi, C.A., Koura, Z.E., Bazzanella, N., Meda, L., Miotello, A.
Pulsed-laser deposition of nanostructured iron oxide catalysts for efficient water oxidation (**2014**) ACS Applied Materials and Interfaces, 6 (9), pp. 6186-6190. DOI: 10.1021/am501021e.

Massimo Cazzanelli (UniTN)

Technical staff at the Physics department, UniTN. Solution-oriented technologist with demonstrated capability to oversee experimentation, to promote quality management and good laboratory practices. Credited with designing and managing highly adaptable laboratories to research studies into optical technology, nanotechnology and space propulsion with practical applications. He authored or co-authored over 60 publications ranging from physics, materials science and engineering (H-factor = 25).

Recent and ongoing projects:

- Progetto PAT Bando Grandi Progetti 2006 "NAOMI Nano on Micro" http://naomi.science.unitn.it/ 2008-12 48months. **Workpackage leader**
- Progetto Fondazione CARIPLO "Studio della non linearità di guide ottiche in silicio periodicamente stressato per nuove sorgenti laser nel medio infrarosso" 2010-12 24months. **Workpackage leader**
- Progetto Fondazione CARIPLO ""Supercontinuo nell'infrarosso ad onde medie da guide d'onda in silicio" 2012-13 24months. **Workpackage leader**
- Progetto PAT Bando Grandi Progetti 2011 "On silicon chip quantum optics for quantum computing and secure communication" 2013-16, 36 months **Workpackage leader**
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Five publications relevant to the project:

1) **M. Cazzanelli***, L. Basso, E. Moser, N. Bazzanella, and A. Miotello, Sensitive magnetic-field detection with size-controlled fluorescent laser-synthesized nanodiamonds, submitted (2019).

2) L. Basso, N. Bazzanella, **M. Cazzanelli**, and A. Miotello, On the route towards a facile fluorescent nanodiamonds laser-synthesis, *Carbon* 153, 148-155 (2019).

3) F. Gorrini, R. Giri, C. E. Avalos, S. Tambalo, S. Mannucci, L. Basso, N. Bazzanella, C. Dorigoni, **M. Cazzanelli**, P. Marzola, A. Miotello, A. Bifone, Fast and sensitive detection of hemoglobin and other paramagnetic species using coupled charge and spin dynamics in strongly fluorescent nanodiamonds, ACS Applied Materials Interfaces 11, 24412-24422 (2019).

4) L. Basso, F. Gorrini, **M. Cazzanelli***, N. Bazzanella, A. Bifone, and A. Miotello, An all-optical single-step process for production of nanometric-sized fluorescent diamonds, *Nanoscale* 10, 5738-5744 (2018).

5) R. Giri, F. Gorrini, C. Dorigoni, C. Avalos, **M. Cazzanelli**, and A. Bifone, Coupled charge and spin dynamics in high-density ensembles of nitrogen-vacancy centers in diamond, Phys. Rev B **98**, 045401 (2018).

Alberto Quaranta (UniTN)

Alberto Quaranta: Full professor of Experimental Physics at the Department of Industrial Engineering. He is involved in research activities on scintillation and nanostructured radiation detectors. The full CV is attached to the project.

Recent and on-going projects:

- **NADIR:** *"NAno Dosimetry of Ionizing Radiation"* (2015-2017) - 5th Commission INFN Experiment - total budget for Trento 20k€.

- **AXIAL**: *"Axial and quasi-axial coherent orientational interactions in crystals"* (2017-2019) - 5th Commission INFN Experiment - total budget for Trento 20k€.

- **ELOFLEX:** *"ELectro-Optical FLEXible detectors for mixed radiation fields"* (2018-2019) – 5th Commission INFN Experiment - total budget 100k€

- **MILA:** *"**M**ateriali **I**nnovativi per rivelazione di **L**uce nell'UV-NIR per **A**utomotive **A**mbiente e Agro-food"* (December 2017 - ongoing) CARITRO Foundation - total budget 95k€.

- **CHEDDAR**: *"CHiplEss RFID RaDiAtion DetectoR" (*May 2019 - ongoing) – ATTRACT 2020 - total budget for DII 30k€.

- **FIRE:** *"Flexible Ionizinig Radiation dEtectors"* (2019 - ongoing) – 5th Commission INFN call- total budget for Trento 100k€.

5 publications relevant to the project:

- *Proton Irradiation Effects on Colloidal InGaP/ZnS Core-Shell Quantum Dots Embedded in Polydimethylsiloxane: Discriminating Core from Shell Radiation-Induced Defects Through Time-Resolved Photoluminescence Analysis*, E. Zanazzi, M. Favaro, A. Ficorella, L. Pancheri, G. F. Dalla Betta, **A. Quaranta**, *The Journal of Physical Chemistry C* 122 (38) 2018, 22170-22177.

- *Versatile and scalable strategy to grow sol-gel derived 2H−MoS_2 thin films with superior electronic properties: a memristive case*, M.V. Nardi, M. Timpel, G. Ligorio, N. Zorn Morales, A. Chiappini, T. Toccoli, R. Verucchi, R. Ceccato, L. Pasquali, E. List-Kratochvil, **A. Quaranta**, S. Dirè, *ACS Applied Materials & Interfaces*, 10 (2018) 34392-34400.

- *Optical properties and pulse shape discrimination in siloxane-based scintillation detectors*, T. Marchi, F. Pino, C. L. Fontana, **A. Quaranta**, E. Zanazzi, M. Vesco, M. Cinausero, N. Daldosso, V. Paterlini, F. Gramegna, S. Moretto, G. Collazuol, M. Degerlier, D. Fabris, and S. M. Carturan, *Scientific Reports*, 9 (2019) 9154.

- *Photoluminescence enhancement of colloidal CdSe/ZnS quantum dots embedded in polyvinyl alcohol after 2 MeV proton irradiation: crucial role of the embedding medium*, E. Zanazzi, M. Favaro, A. Ficorella, L. Pancheri, G.F. Dalla Betta, **A. Quaranta**, *Optical Materials* 88 (2019) 271-276.

- *Radiation-induced optical change of ion-irradiated CdSeS/ZnS core-shell quantum dots embedded in polyvinyl alcohol*, E. Zanazzi, M. Favaro, A. Ficorella, L. Pancheri, G. F. Dalla Betta, **A. Quaranta**, *Nuclear Instruments and Methods B* 435 (2018) 327-330.

8. The project is relevant for the following Q@TN work-package(s):

- **WP1:** Fundamental quantum science, *area of action:* fundamental quantum physics, quantum optics

- **WP2:** Quantum communications, *area of action:* Quantum number generators, Quantum key distribution

- **WP3:** Quantum computing, *area of action:* Single photon sources for quantum computing

- **WP5**: Future sensors and metrology, *area of action:* micromagnetic sensors

9. Description of the project

Activities, objectives, deliverables, estimated total cost, available resources to sustain the activity, etc. (max two pages in Times New Roman 11, excluding references)

The production of fluorescent nano-diamonds with room-temperature magnetic sensing capabilities is one of the most challenging tasks in quantum technologies for sensors, metrology advanced applications as well as for the comprehension of fundamental aspects of nonclassical properties of light. This problem is generally tackled by following a sequence of poorly controlled procedures that do not straightforwardly lead to the manufacturing of N-doped nanodiamonds characterized by a well established size and by a nitrogen-vacancy (NV) specific content and tailored pattern.

In this regard, the *Laboratorio Idrogeno Energia Ambiente (IdEA)* of the University of Trento has gained significant expertise in the fabrication of nano-diamonds up to the stage of quantum sensor applications using a technique based on pulsed laser ablation of graphite (https://www.leggo.it/societa/scienze/trento_diamanti_universita_acqua-2113262.html o https://www.galileonet.it/diamanti-bicchiere-acqua-laser-ricerca/). In particular, by ablating commercial pyrolitic graphite in liquid environment, such as in water and/or in liquid nitrogen, by a high-fluence laser, *Idea Lab* has been able to synthesize high-quality fluorescent nano-diamonds. At variance with previous approaches to nano-diamond fabrication, this method is characterized by only one-step and does not need any post-processing of the nanomaterials, except for possible residual graphitic layers,which makes it cost-effective and facile. Most importantly, these nano-diamonds show interesting magnetic-dependent fluorescent properties, basically derived by the controlled incorporation of NV optically active defects inside the diamond matrix. Despite the significant scientific track (see reference list) already produced by this recently started research activity, the anticipated disruptive nature of this synthesis route of nanodiamond-based quantum sensors for significant future widening of this technology is hampered by the low-yield of the production process. The magnetic-sensing capabilities of the nanodiamonds manufactured in the *Idea Lab* are such that one can readily detects few tens of $\mu T/\sqrt{(Hz)}$ in simple opto-magnetic schemes (see Figure 1, unpublished and **confidential**), such as in the so-called continuous-wave-electron-spin-resonance (CW-ESR) that only needs a synchronous radiofrequency and an optical pump.

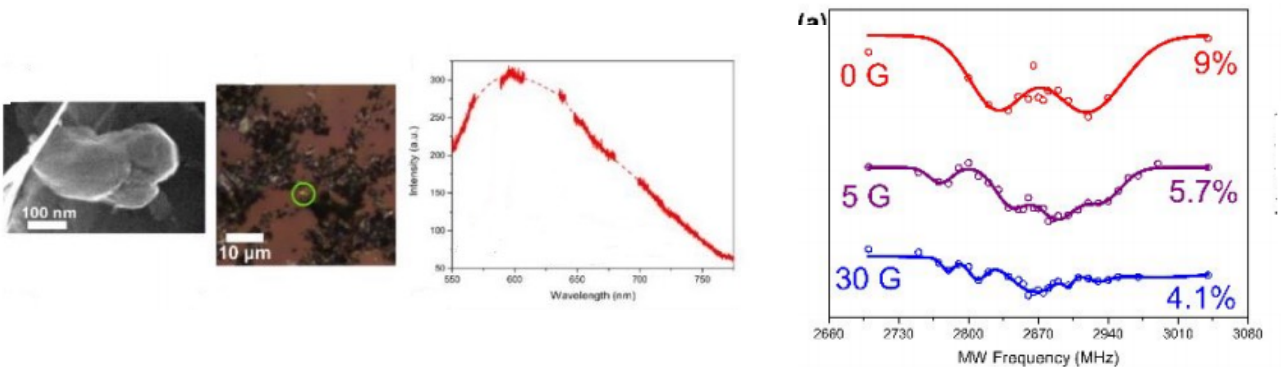

Figure 1: From left to right: SEM micrography, optical imaging of nanodiamonds (with the surrounding residual graphitic shells) and atypical micro-photoluminescence spectrum.

Rightmost panel: optically detected magnetic resonance (ODMR) spectra on NV centers in pulsed laser deposited nanodiamonds. The typical fingerprint resonance at 2.87 GHz unambiguously shows the presence of magnetic sensitive NV^- centers. Analysis of these data (submitted 2019) reports a "*state-of-the-art*" CW-ESR magnetic detection sensitivity of $18 \pm 5\mu T/\sqrt{Hz}$.

In particular, NV-related optically detected magnetic resonance spectra (ODMR) can be detected on randomly oriented ensembles of pulsed laser ablated nanodiamonds, resolving (for example via the contrast-determination of the spectra) very feeble magnetic fields.

⇨ This project is aimed at studying novel approaches to overcome the production yield bottleneck of these nano-devices and to boost the graphite-to-nanodiamonds transformation rate towards mass scale manufacturing of very sensitive, clean magnetic nanosensors. Of course, this task critically relies on a better understanding of nitrogen incorporation under laser ablation conditions. We plan to achieve this thorough understanding via three concurrent routes.

- First we propose to increase the repetition rate of the high fluence laser ablation process, resulting in an increase of production of nano-diamonds, roughly proportional to the laser fluence. 100 Hz at the same fluence are accessible with the existing and available apparatuses. Higher repetition rates could be accessed in external Laboratories. The increase in the production rate has to take into account the effects due to the agglomeration processes of the nanoparticles, giving rise to screening phenomena of the laser pulses interacting with the graphite matrix. For this reason, specific configurations of the apparatuses must be analyzed, possibly also providing for a flow of selected colloidal solutions. Moreover, doped nano-diamonds produced with the new procedures needs to be characterized with optical spectroscopy, microscopy and structural methods in order to understand how the screening phenomena can affect the formation of the nano-particles and of the emitting centers.
- Second, theoretical and computational modelling will be used to understand, and thus optimize, the mechanisms underlying the nitrogen incorporation at the nano-diamond formation stage. The processes of incorporation of nitrogen atoms into the nanoparticles, given the non-equilibrium conditions at which they occur, are not simply deducible from the normal phase diagrams (valid for equilibrium conditions) but occur through metastable phases that must be studied in detail to understand their relevant time scales also with the possibility of incorporating a number of nitrogen atoms above the thermodynamic limits. The overcoming of the solubility limits is a significant objective in this sector in order to increase the efficiency of quantum sensors that operate on the basis of the optical properties of the N-V centers and a proper modelling is of paramount importance for the development of the process..
- Third, we will develop an optimized reaction work-up procedure for cleaning the residual graphitic shells. Understanding the formation mechanisms of these shells will help in the development of cleaning methodologies that could also be adopted during the same production process.

To achieve these goals our team comprises: a strong fabrication component; quantum scientists with a demonstrated ability to combine different ab-initio and multiscale techniques at different times and length scales to model the chemical-physical processes underlying the growth; spectroscopic characterization methods for the analyses of the emitting centers; leading scientific expertise in connection with technological delivery required to develop and use these new quantum sensors with magnetic capabilities; on-field expertise in opto-magnetic development of innovative scientific apparatuses.
In particular, the research activity of this project will be pursued on a two-fold level. First, the PhD student will be asked to develop suitable experimental deposition strategies to increase the nano-diamonds production yield (now limited to ~ few μg), for example by increasing the high-fluence laser repetition rate by depositing diamond nanopowders (up to 100 Hz within IdEA Laboratory and >100 Hz in external high power laser facilities collaborating with the research consortium). In this regard, the expected result is the development of an accomplished and reliable method for producing milligrams of graphite-free NV-doped nano-diamonds. Furthermore, testing of their magnetic sensing capabilities will be pursued in order to compare in terms of sensing capabilities our systems with state-of-the-art devices (see Ref [1]). Due to the reliability and reproducibility of the overall manufacturing process we expect that our systems perform better than those existing in this respect. The manufactured samples will be analyzed with time resolved optical spectroscopy and microscopy techniques. Optical spectroscopy will be fundamental for characterizing the properties of the NV luminescent centers, while a recently acquired TEM will be used for the characterization of the structural properties of the nano-particles.

Second, he/she will be able to interface with the computational scientists participating in this project and modelling the nitrogen intercalation mechanisms in the liquid carbon co-existing with vapour carbon in the phase-explosion scenario induced by the high-fluence laser ablation of graphite. In particular, he/she will get insights on first-principles and multiscale simulations, based on molecular dynamics and kinetic Monte Carlo, to calculate e.g. the nitrogen dissociation rate and the energy barriers to intercalate within the nano-diamond lattice and form the vacancy. This theoretical analysis is aimed also at finding optimal experimental deposition parameters in order to fine-tune the NV-concentration in the nano-diamonds and to control efficiently the nano-diamonds tail distribution (which, in our case, is intrinsically superior-limited to ∼100 nm, see Refs. [2, 6]).
For all aspects concerning numerical modelling, the use and development of the complex code suites to perform electronic structure and molecular dynamics simulations, the hired resource will rely on the support and the results provided by the quantum scientists based at the European Center for Theoretical Studies in Nuclear Physics and Related Areas (ECT*). ECT* will collaborate in the development of the codes for the theoretical analyses and the Department of Industrial Engineering for the optical characterization.
In all the experimental activities the student will be assisted by the technicians and the staff at the Department of Physics, having a long lasting experience in both deposition as well as opto-magnetic characterization and device fabrication.

List of deliverables:

1. By the end of the first year (**M12**) of activity we are confident to achieve the optimized production of at least 1 mg of nano-diamonds (plus graphitic residuals) using an efficient physico-chemical cleaning procedure of graphite removal.
2. At **M18** we plan to improve the cleaning procedure by increasing the ratio of nano-diamonds/graphite. The figure of merit to achieve is to get basically graphite-free nano-diamonds (e.g. 95% nanodiamonds, 5% graphite).
3. By the end of the second year (**M24**) we will carry out computer simulations on the nitrogen incorporation in the nano-diamond lattice during the high-temperature, high-pressure fast processes occurring during the laser ablation of graphite in liquid confining environments.
4. At **M30** we will deliver the installation of an optimized ODMR laboratory capable to detect optically the magnetic resonance from micrometric sized clusters of the laser-synthesized nano-diamonds.
5. At **M36** we will demonstrate (Lab demonstrator) a scalable opto-magnetic sensing scheme relying on solid state 532 nm laser and sCMOS detection.

Available resources to sustain the activity:

1. *Proof-of-principle* experimental lay-out (see Ref [1]) of a locally available ODMR apparatus. This apparatus can be readily and cost-effectively developed to measure and

image ODMR signals from micrometric regions under green laser irradiation and radiofrequency co-pumping. A scheme of such apparatus is sketched in Fig. 2.

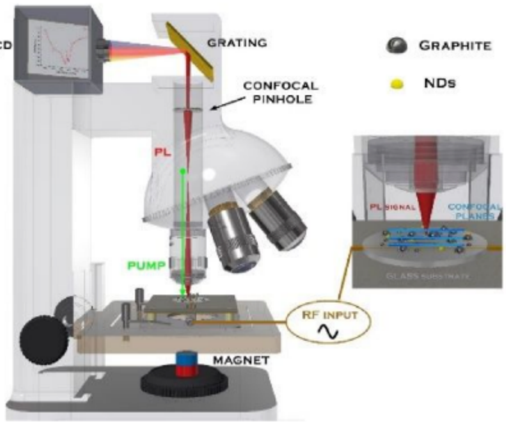

Figure 2: Confocal ODMR imaging apparatus available to the research consortium.

2. High throughput hardware and simulation software tools at ECT* to carry out the *ab-initio* and molecular dynamics calculations.
3. High-fluence (up to 100 Hz) UV excimer laser for the liquid-confined laser ablation production of nano-diamonds.
4. Local physico-chemical expertise in diamond cleaning and (nano-)manipulation.
5. High-resolution transmission electron microscopy

References

1) M. Cazzanelli, L. Basso, E. Moser, N. Bazzanella, and A. Miotello, Sensitive magnetic-field detection with size-controlled fluorescent laser-synthesized nanodiamonds, submitted (2019).

2) L. Basso, N. Bazzanella, M. Cazzanelli, and A. Miotello, On the route towards a facile fluorescent nanodiamonds laser-synthesis, *Carbon* 153, 148-155 (2019).

3) F. Gorrini, R. Giri, C. E. Avalos, S. Tambalo, S. Mannucci, L. Basso, N. Bazzanella, C. Dorigoni, M. Cazzanelli, P. Marzola, A. Miotello, A. Bifone, Fast and sensitive detection of hemoglobin and other paramagnetic species using coupled charge and spin dynamics in strongly fluorescent nanodiamonds, ACS Applied Materials Interfaces 11, 24412-24422 (2019).

4) L. Basso, F. Gorrini, M. Cazzanelli, N. Bazzanella, A. Bifone, and A. Miotello, An all-optical single-step process for production of nanometric-sized fluorescent diamonds, *Nanoscale* 10, 5738-5744 (2018).

5) Luca Basso, Federico Gorrini, Nicola Bazzanella, Massimo Cazzanelli, Carla Dorigoni, Angelo Bifone, and Antonio Miotello, The modeling and synthesis of nanodiamonds by laser ablation of graphite and diamond-like carbon in liquid-confined ambient, *Appl. Phys. A* 124, 72 (2018).

6) F. Gorrini, M. Cazzanelli, N. Bazzanella, R. Edla, M. Gemmi, V. Cappello, J. David, C. Dorigoni, A. Bifone, and A. Miotello, On the thermodynamic path enabling a room-temperature, laser-assisted graphite to nanodiamond transformation, *Scientific Reports* 6, 35244 (2016). Nature Publishing Group.

10. Interdisciplinary aspects

Teams involved, interdisciplinary competences, role of the requested position for strengthening new co-operations within Q@TN (max one page).

This project involves the development of ultra-sensitive instrumentation based on quantum effects to optically detect magnetic resonance signals. To understand the physical and chemical processes involved in the materials fabrication a strong expertise in both basic science and technology is required. This project is thus based on a strong synergetic effort of the experimental and synthesis team of UniTN (led by Antonio Miotello), of the team working on optical spectroscopy at the Department of Industrial Engineering (Alberto Quaranta), and of the computational many-body physics division at ECT* (Simone Taioli). All the teams involved in this project have international recognized reputations on electronic structure and molecular dynamics simulations of carbon based (nano-)structrures and on laser ablation of functionalized materials, respectively.

In particular, the skills of the different teams can be summarized as follows:

- The team of Antonio Miotello at UniTN has a long-lasting experience in materials science with particular emphasis on the technological exploitation of laser ablation processes and plasma physics. Noticeable to this project is the strong expertise of this team in the field of the physical-chemistry of nanomaterials synthesis and processing, as well as of the advanced optical characterization of solid state (nano-)materials. Recently the group has extended the characterization tools towards opto-magnetic spectroscopy like ODMR (CW-Electron Spin Resonance).

- Concerning the characterization techniques, the team of Alberto Quaranta at the Department of Industrial Engineering has a documented expertise in the optical characterization of nanostructured materials and quantum dots. By means of the facilities of the Department of Industrial Engineering, Alberto Quaranta will also support the experimental investigations also through TEM and X-ray diffraction measurements on the produced samples.

- A further aspect of this project will be the use and development of mathematical and computational methods in electronic structure theory and multiscale techniques, in particular related to the accurate modelling of nitrogen dissociation and intercalation in the nanodiamond matrix at experimental conditions. In the team these topics will be supervised by Dr. Simone Taioli at ECT*. The ECT* team has a broad expertise in the solution of the many-body problem in condensed matter, with particular emphasis on carbon nanostructures, scattering theory, and the dynamic evolution of molecules and solids. The team members routinely use a variety of techniques at different level of accuracy, from mean-field to strongly correlated methods, also developed in-house in custom programs that will allow an accurate modelling of this problem in the relevant experimental conditions.

To be successful, this project requires a tight collaboration and interaction of these three teams. In this way the theoretical and the experimental partners can mutually sustain each other. The hired resource will be involved mainly in the experimental activity but has to be able to interact efficiently with the theoretical group. In this way not only she/he will understand the theoretical background necessary to implement the complex mathematical equations ruling the nitrogen incorporation process within the extreme thermodynamical conditions induced by the high-fluence laser interaction with the graphite target, but will also have a full understanding/control of the experimental aspects related to i) find viable experimental solutions to optimize the manufacturing of magneto-optically functionalized nanodiamonds, ii) characterize them, and iii) devise possible technological and practical applications of these systems.
The funding from Q@TN will reinforce the collaboration between these three groups, and foster the development of *cutting-edge* technologies critical for many promising fields of quantum science and beyond. In addition it will give a unique opportunity to the hired resource to get trained in up-to-date technology and physics. She/he will surely benefit from a strong interdisciplinary environment and by the end of his/her professional path will be highly skilled in the development of extremely sensitive, biocompatible, room-temperature magnetic quantum sensors. Finally, he/she will be also pivotal for initiating experimental-theoretical cross-fertilization aimed at opening, inside the Q@TN research framework, a quantum sensing applicative research line.

11. Relevance of the project for quantum science and technology
Significance of the project objectives for the advances of quantum science and technology in a broad sense, at the national and international level. Perspectives for a future development of the activity (max one page).

To achieve its goals as well as to translate academic work on quantum physics into new products and services, the second quantum revolution must rely on technologies that use equipment such as highly stabilised laser systems, magneto-optical and solid state devices. To create and manipulate,

effectively and reliably, quantum effects to outperform classical technological platforms, one needs both novel quantum algorithms but also serious advancement in the existing hardware operating in quantum secure communications, quantum sensing metrology and quantum imaging. This proposal aims to bridge the gap between fundamental physics and technological advancements by developing a peculiar route to use ensembles of nano-diamonds containing NV centers as room temperature, temperature-independent, magnetic quantum sensors. The perspective experimental and theoretical developments of this activity rely on the magnetic sensing properties of NV centers in the nanodiamonds (which can be effectively experimentally decoupled from the temperature sensing ones) as well as in their local electric/strain fields sensing capabilities (see Ref. [4]). While this approach builds upon the long experience of the UniTN team in sensor design and production, it is strikingly innovative because it relies on collective magneto-optical effects (see Ref. [1,2,3]) of NV-doped nano-diamond random ensembles grown by laser ablation in liquid environment. The nano-diamonds act as magnetic quantum-sensors at odds with the widely used N-implanted bulk diamonds. We are confident that this proposal will implement a reliable route towards real biocompatible, as well as *space-compliant*, magnetic, cheap and temperature-independent sensors. We believe that this research line will make it possible to open new directions within the Q@TN consortium by developing a strong theoretical and experimental expertise in the field of magnetic sensing. Thus, this project will help to launch the Q@TN consortium at the forefront of the international efforts in the exciting physics at the high sensitivity frontier in both national and international scenarios and to build a role in future experiments that will surely constitute a major part of the European flagship in quantum science and technology.
This project represents therefore a strategic investment for the Q@TN initiative within an important field of science and technological development.

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