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DEGLI STUDI  
DI PADOVA

UNIPD and UNIVE for NEST - Spoke 9

Innovative materials for solar energy conversion and storage



## WP 9.0: Coordination

### WP 9.1: Innovative synthesis of materials for energy applications

- T9.1.1. Strategies to boost the catalytic efficiency of materials
- T9.1.2. Engineering of materials with improved chemico-physical properties
- T9.1.3. Self-assembly of supramolecular and hybrid nanostructured systems
- T9.1.4. Materials operating under non-standard, severe and extreme conditions
- T9.1.5. Multifunctional, composite and low-dimensional materials

### WP 9.2: Efficient preparation of sustainable materials

- T9.2.1. Green preparation protocols and materials
- T9.2.2 Design strategies for recyclable materials
- T9.2.3 LCA and new regulations for the development and use of advanced materials in a circular economy approach

### WP 9.3: New production processes of materials for energy applications

- T9.3.1 Innovative manufacturing, nanofabrication and consolidation processes
- T9.3.2. Surface functionalization, interface processing, arrays
- T9.3.3 Processing methods to extend materials lifetime

### WP 9.4: Materials characterization and testing

- T9.4.1: Advanced structural and morphological characterization techniques
- T9.4.2: Optical, electrochemical, electronic properties
- T9.4.3: Magnetic, thermal and transport properties
- T9.4.4: In situ, operando characterization and testing of materials

### WP 9.5: Advanced computational modelling for materials development

- T9.5.1 Computational methods and modeling to predict materials structure and properties
- T9.5.2 Advanced computational approaches for improving materials efficiency and performance

### WP 9.6 Dissemination and Communications



Marcella Bonchio, Nano & Molecular Catalysis Laboratory,  
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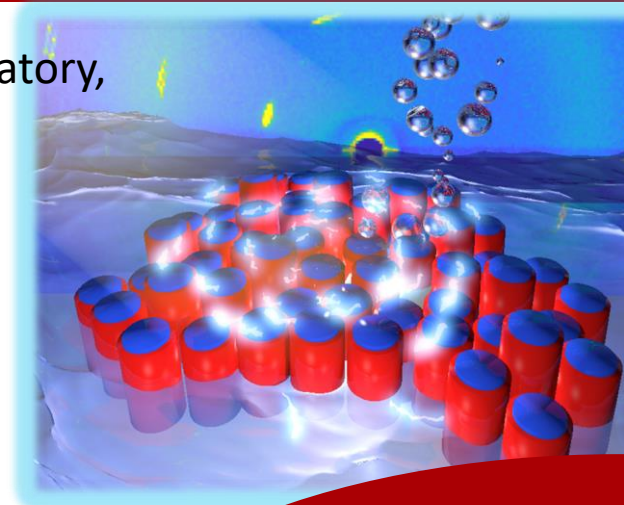
Dept of Chemical Sciences, University of Padova

Daniele Rosa-Gastaldo (RTDa\_NEST)

Leonardo Cognigni (PhD)

Ilaria Crea (PhD)

Jintao Liu (PhD)



- photo(electro) catalysis mechanisms @interfaces
- supramolecular catalysis for artificial photosynthesis
- Organic semiconductors and fabrication of photonic electrodes
- **Synthesis:** Organic and Inorganic reaction protocols for molecular building blocks and materials doping
- **Characterization:** NMR, MS and optical spectroscopies (FTIR, Raman, Uv-Vis, Fluorescence) for probing the molecular structure and product analysis
- **Properties:** PEC efficiency and selectivity for solar fuel production

- 9.1 Innovative synthesis of materials for energy applications
- 9.3 New production processes of materials for energy applications

1. Nature Chemistry (2019), 11, 146 <https://doi.org/10.1038/s41557-018-0172-y>
2. Nature Commun. (2020) 11, 41. <https://doi.org/10.1038/s41467-019-13759-1>
3. J. Am.Chem.Soc. (2022) 144,14021. <https://doi.org/10.1021/jacs.2c05857>
4. Nature Catalysis (2023) 6, 657–665 <https://doi.org/10.1038/s41929-023-00992-7>



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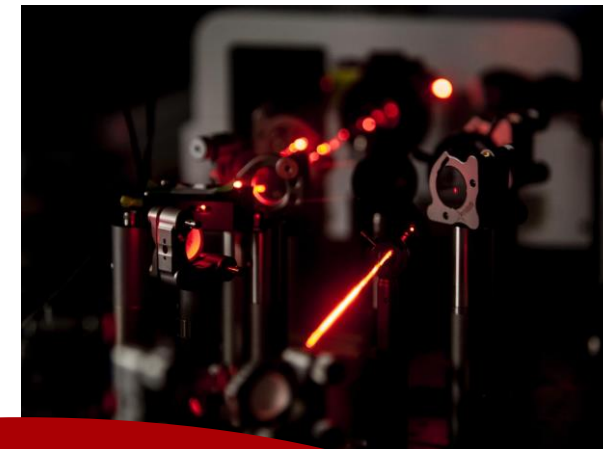
# UNIPD for NEST, spoke 9



Multidimensional  
and Ultrafast Optical  
Spectroscopy Group



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- Time-resolved techniques (from fs to ms timescale)
- Femtoseconds dynamics;
- Multidimensional coherent spectroscopies;
- photophysical and dynamical characterization of light-harvesting and energy transport processes;
- optical properties of functional nanomaterials;
- mechanisms of photo-activated chemical reactions

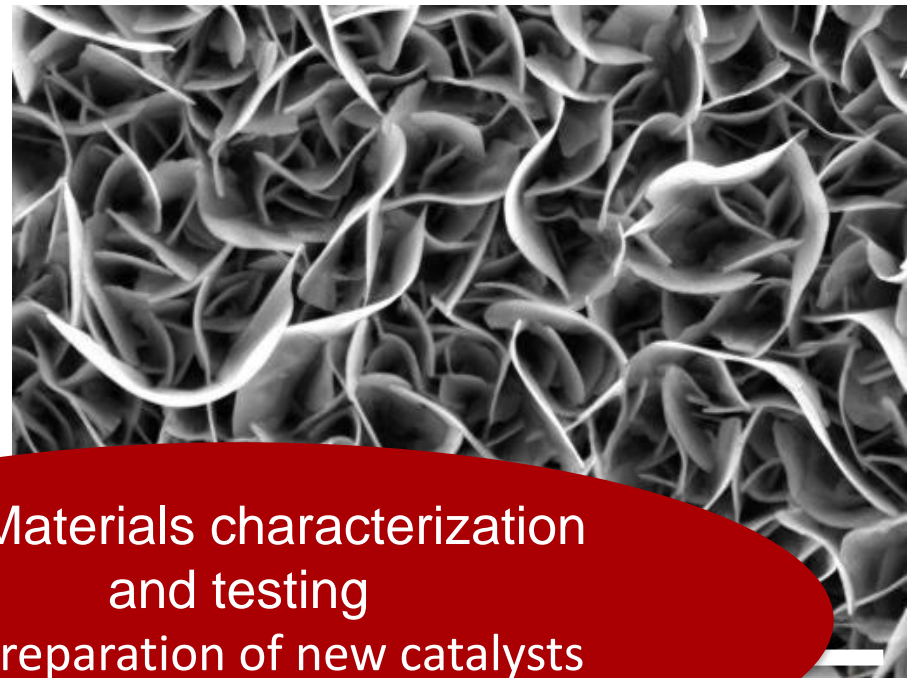
## 9.4 Materials characterization and testing

1. Adv Energy Mater (2022) 2103556  
<https://doi.org/10.1002/aenm.202103556>
2. J Phys Chem C 125 (2021) 13096  
<https://doi.org/10.1021/acs.jpcc.1c02693>
3. J Phys Chem Lett 12 (2021) 3983  
<https://doi.org/10.1021/acs.jpcllett.1c00822>



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Paola Ragonese PhD  
Bibiana M. Fernandez Perez RTDa



- Nanostructured films for light-driven OER and HER
- Charge transfer@interfaces
- Multi-approach characterization
- Synchrotron radiation-based techniques
- **Synthesis:** PVD, evaporation, patterning, atmospheric pressure plasma
- **Characterization:** SEM-related, AFM-related, in-situ GIXRD, Raman, FTIR, optical spectroscopies (time resolved photoluminescence)
- **Properties:** PEC and related spectroscopies (EIS, IMPS, IMVS)

## 9.4 Materials characterization and testing

- 9.1 Preparation of new catalysts
- 9.3 New production processes

1. Appl. Surf. Sci. 596 (2022) 153552.  
<https://doi.org/10.1016/j.apsusc.2022.153552>
2. Appl. Surf. Sci. 439 (2018) 876.  
[10.1016/j.apsusc.2018.01.121](https://doi.org/10.1016/j.apsusc.2018.01.121)
3. Appl. Surf. Sci. 513 (2020) 145779.  
<https://doi.org/10.1016/j.apsusc.2020.145779>



# UNIVE (affiliate) for NEST, spoke 9



Marco Bortoluzzi

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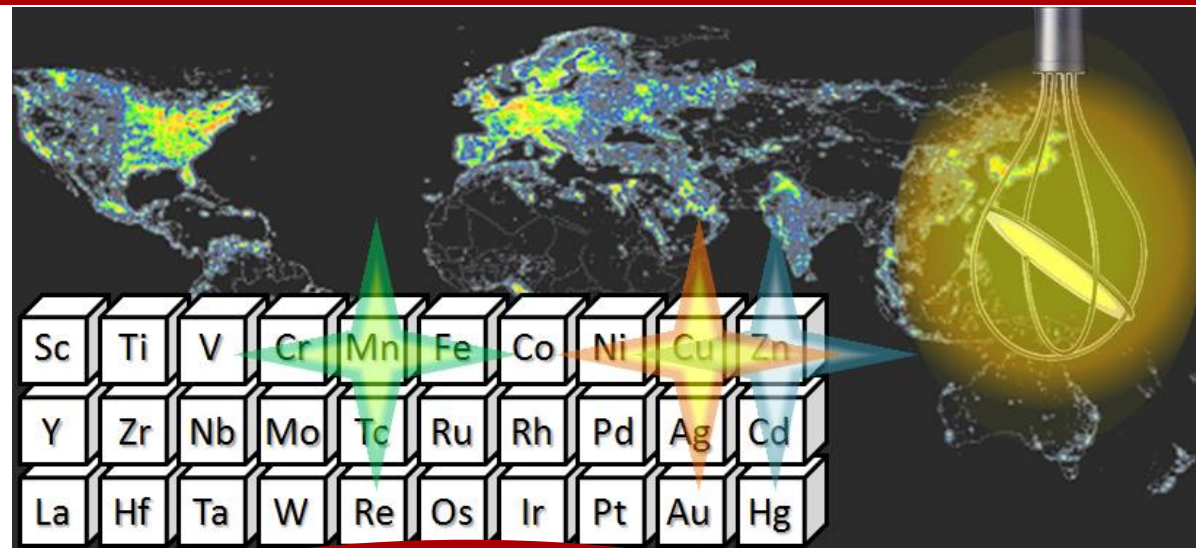
Collaborations

Jesús Castro (Vigo University, Spain).

Valentina Ferraro (KIT, Germany).

Students: Domenico Piccolo, Matteo Donati

- Coordination chemistry
- Synthesis and characterization of luminescent coordination compounds based on earth-abundant elements for energy conversion.
- Steady-state and time-resolved luminescence measurements.
- Computational simulations (DFT, TD-DFT) for energy-converting molecular systems



9.4 Optical properties  
9.5 Advanced computational methods

1. New J. Chem. 46 (2022) 18938-18951. <https://doi.org/10.1039/D2NJ03165E>
2. Dalton Trans. 50 (2021) 3132-3136. <https://doi.org/10.1039/D1DT00123J>
3. Dalton Trans. 49 (2020) 7525-7534. <https://doi.org/10.1039/D0DT01659D>



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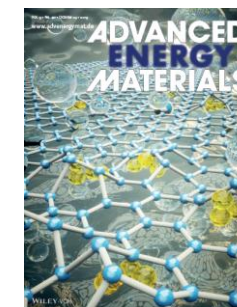
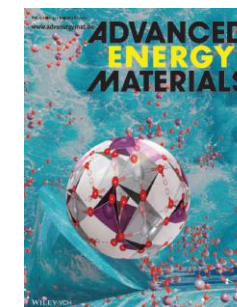
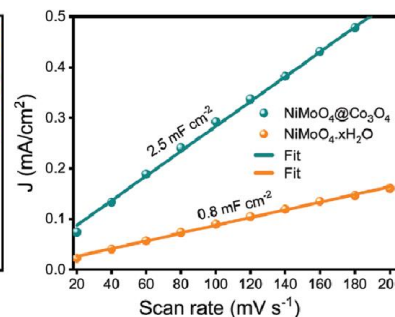
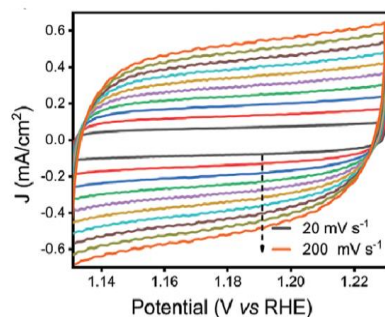
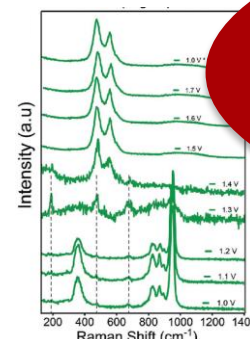
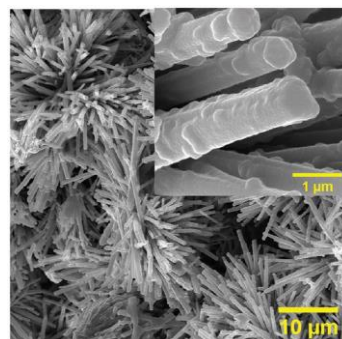
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Tofik Ahmed Shifa - RTD B  
Kassa Belay Ibrahim - RTD A  
Anastasiia Taranova - PhD student

- 0-1-2 D nanomaterials for water splitting / hydrogen production
- Confined catalysis
- Operando spectroscopies

## Available techniques:

- PVD growth
- Operando Raman
- Atomic force microscopy
- Optical spectroscopies
- Rutherford backscattering



9.1 Preparation of new catalysts  
/ Confined catalysis  
9.4 Materials characterization  
and testing

[NiMoO<sub>4</sub>@Co<sub>3</sub>O<sub>4</sub> Core-Shell Nanorods: In Situ Catalyst Reconstruction toward High Efficiency Oxygen Evolution Reaction](#)

G Solomon, et al. Adv En Mater 11 (2021) 2101324

[Facile Electron Transfer in Atomically Coupled Heterointerface for Accelerated Oxygen Evolution](#)

KB Ibrahim, et al. Small 19 (2023) 2204765

[Interfacing CrOx and CuS for synergistically enhanced water oxidation catalysis](#)

TA Shifa, et al. Chem Eng J 453 (2023) 139781

# UNIPD for NEST, spoke 9

optically detected  
2DES setup



Photocurrent detected  
2DES setup

new laser source  
(Carbide+NOPA) purchased  
with PNRR funds:

- 50KHz rep rate
- Tunable from 200 to 750 nm
- 10-20 fs pulse duration

T9.4.1: Advanced structural and  
morphological characterization  
techniques

T9.4.2: Optical, electrochemical,  
electronic properties





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**Alberto Vomiero**

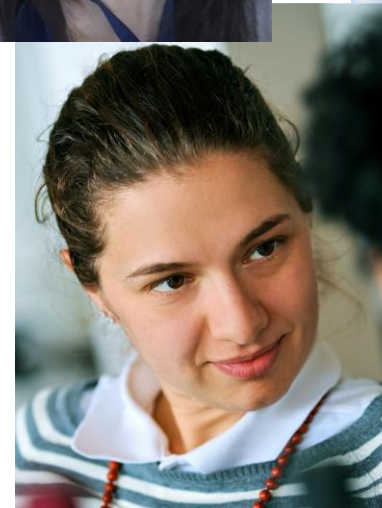
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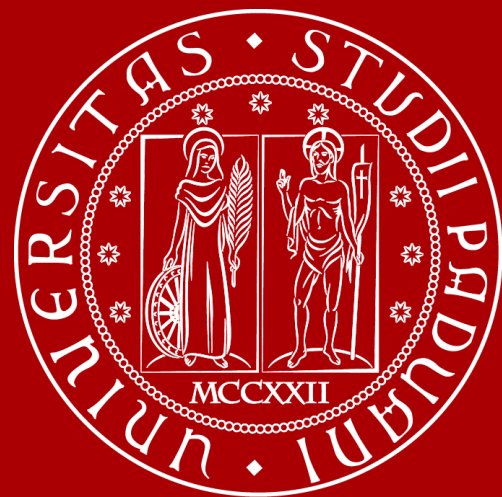
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