# Seminar

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## *Diamond molecular interfaces for solar energy conversion*

**Tuesday, 25 February 2025, h. 11.00**

**Wataghin Room, Physics department, via Pietro Giuria 1, Torino**

***Abstract***:

Modern concept and devices for energy conversion including photovoltaic solar cells continue to explore the idea of using molecules, polymers and nanomaterials in key parts of such systems. There are several reasons for this: shorter time to return the energy used for device fabrication, lower production and deployment costs, principally better power output under low-light or diffuse light conditions such as in hazy weather, building integration or indoor applications, and last but not least material and energy independence of Europe. In spite of many advances in the past decades, the technology still need improvements in terms of efficiency, materials cost, and long-term stability for scaling up its production and practical applications. In all these aspects, diamond-based hybrid systems may have an immense potential, which is still mostly underexplored. Diamond as technological material is abundant, inexpensive and non-toxic. Our long term research shows that diamonds can advantageously act as more stable inorganic electron acceptors, light trapping enhancers, interface for more efficient charge separation, transparent electrodes for charge transport, and more. A nanocomposite fabrication technology with polypyrrole (PPy) and nanodiamond (ND) is presented. The formation, pronounced material interaction, and photovoltaic properties of ND-PPy composites are characterized down to nanoscale by atomic force microscopy, optical spectroscopies, Kelvin probe, and electronic transport measurements. NDs with different surface terminations (hydrogenated, oxidized, poly-functional) assemble PPy oligomers in different ways, leading to different optoelectronic properties. Infrared spectroscopy shows a tight nanoscale interaction between ND and PPy in the composites, which explains enhanced optical absorption and more efficient charge generation. Combination of both oxygen and hydrogen functional groups on the nanodiamond surface appears to be the most favorable. Photovoltage shows that NDs act as electron acceptors. Theoretical calculations of the structure and electronic properties show HOMO-LUMO separation in the ND-PPy complex and elucidate mechanism of exciton dissociation. Somewhat counterintuitively, hydrogenated NDs also work best as electron transporting layers instead of ZnO or SnO when combined with polymer solar cells. Analysis of energetic levels of hydrogenated NDs of various origin and their conductivity helps understand these effects.

*References*

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# Biography

Bohuslav Rezek is a professor of Applied physics and the head of Physics dept. at the Faculty of Electrical Engineering of the Czech Technical University in Prague.

He graduated from Physics at the Faculty of Mathematics and Physics at the Charles University in Prague in 1996 and he continued at the Czech Academy of Sciences (CAS) in the group of Dr. Jan Kočka with PhD study on charge transport in amorphous and microcrystalline silicon with high lateral resolution by using scanning probe techniques. During his PhD he also had several research stays in the group of Prof. Martin Stutzmann at the Walter Schottky Institute, Technical University Munich. There he worked with Dr. Christoph Nebel on development of large grain silicon thin films using interference laser crystallization of amorphous silicon layers and on their investigation by laser beam induced currents with a sub-micrometer lateral resolution, with a special view to optical and electronic properties of grain boundaries.

After receiving PhD degree in 2001, he continued in the group of Prof. Stutzmann as a postdoctoral researcher on the project for diamond devices and sensors where he focused on a study and modification of hydrogen terminated diamond surfaces and their electrolytic interfaces. In 2002 he joined the Nanotechnology Group at the Swiss Federal Institute of Technology, where he worked on guided assembly of colloidal nanoparticles at solid state surfaces. Since 2004 he worked at the Diamond Research Center of AIST in Tsukuba, Japan, doing research on surface (bio)-functionalized diamond devices.

In 2006 he became research group leader and Purkyně Fellow at the Institute of Physics CAS in Prague, Czech Republic. In 2013 he habilitated in the field of Applied physics. Since 2015 he became also a head of Physics dept. at the Faculty of Electrical Engineering of the Czech Technical University in Prague. In 2019 he became full professor there. Among other duties he chairs the doctoral study program of Applied Physics and governmental evaluation panel of Natural Sciences.

His research team is focused on nano-interfaces of semiconductors and organic materials towards opto-electronic and bio-electronic applications. His main interests lie in characterization and modification of material, electronic, and chemical properties by local probe techniques as well as in assembly of organic and inorganic nanostructures. Experimental studies are complemented by simulations on atomic and molecular scale.

He is the author or co-author of over 200 scientific articles in international peer-reviewed journals that were cited more than 4000 times as well as of book chapters (10) and patents applications (6). More details can be found at https://scholar.google.cz/citations?user=mb1lXcUAAAAJ.