**Laboratory of computational chemistry**

completed by responsible coordinator of equipment

**Equipment:**  Laboratory of computational chemistry

**No. of Equipment:** UJEP 34

**Responsible coordinator:** Mgr. David Poustka

**Name of Institution:** Jan Evangelista Purkyně University in Ústí nad Labem

**Address of Institution:** Pasteurova 1, 400 96 Ústí nad Labem, Czech Republic

**E-mail:** davidpoustka@seznam.cz

**Telephone:** +420 604 214 277

**Homepage:** https://www.physics.ujep.cz/cs/personalni-slozeni/rndr-marek-maly-ph-d/

**Contact person (operator):** Mgr. David Poustka

**E-mail:** davidpoustka@seznam.cz

**Telephone:** +420 604 214 277

**Equipment Description**

This laboratory is composed of two computer clusters for high performance computing. The newer cluster consists of 18 nodes "DELL PowerEdge T640 Server", providing a great background especially for more demanding parallel computations. Each node is equipped with 2 Intel Xeon Gold 6240 processors and 192 GB (16 nodes) or 384 GB (2 nodes) RAM. In addition, 10 nodes are equipped with four GeForce RTX 2080 Ti graphics cards for GPU or GPU/CPU calculations. The older cluster consists of 9 older nodes "Dell PowerEdge R720" (2x Intel Xeon E5-2695 v3, 128 GB RAM) and two newer nodes "TYAN - GPU Server FT48TB7105" (2 x Intel Xeon Gold 6240, 192 GB RAM) which are moreover equipped also with 3 x GeForce RTX 2080 Ti for GPU accelerated calculations.

**Specification of expertise relevant to NanoEnviCz workpackages:**

|  |  |
| --- | --- |
| **WP3 SYNTHESIS AND DESIGN OF NEW MULTIFUNCTIONAL NANOMATERIALS FOR ENVIRONMENT PROTECTION** | |
| Conceptually new nanostructured materials with the potential for application in innovative technologies | x |
| Computer aided nanomaterials design | x |
| Low dimensional materials and their composites (carbon dots, nanotubes, graphene derivatives) | x |
| Nanofibers |  |
| Magnetic hybrids |  |
| Metal and metal oxide NPs |  |
| Redox active nanomaterials |  |
| Nanomaterials for biomedical applications | x |
|  | |
| **WP4 HETEROGENEOUS CATALYSIS FOR ENVIRONMENTAL PROTECTION** | |
| Nanomaterials for catalytic degradation of pollutants in water, soil and air |  |
| Nanostructured heterogeneous catalysts for abatement of pollutants from industrial processes and automotive transport | x |
| New “clean” catalytic processes for chemical production |  |
|  | |
| **WP5 NOVEL NANOMATERIALS AND TECHNOLOGIES FOR SUSTAINABLE PRODUCTION** | |
| Processes and technology for sustainable energy and chemical production |  |
| Catalytic processes for transformation of natural gas to liquids |  |
| Nanomaterials for utilization of renewables; Magnetically separable green catalysts |  |
|  | |
| **WP6 EFFECTIVE PHOTOCATALYTIC TECHNOLOGIES** | |
| Mastering nanomaterials for photocatalysis |  |
| Effective photocatalytic processes |  |
| Photovoltaic paints |  |
| Functional surfaces for environmental protection |  |
| Hybrid materials combining photocatalysts and heterogeneous catalysts |  |
| Thin photocatalytic films for direct solar splitting of water |  |
|  | |
| **WP7 NANOTECHNOLOGY FOR TRAPPING AND CHEMICAL DEGRADATION OF POLLUTANTS** | |
| Nanomaterials for sorption | x |
| Natural based nanomaterials produced by “green” technology |  |
| Reactive sorbents for degradation of pesticides and highly toxic agents |  |
| Degradation of chemical warfare agents |  |
| Analysis of filtering capabilities of nanomaterials |  |
| Elimination of radionuclides contamination |  |
| Modified nanofiber filters; Advanced antimicrobial filters/membranes | x |
| Nanoiron for groundwater and waste water treatment |  |
| Nano-trapping of heavy metals |  |
|  | |
| **WP8 SENSING AND MONITORING OF POLLUTANTS** | |
| Efficient sensing of pollutants |  |
| Biosensing by new devises |  |
| Application of new sensors in monitoring of pollutants |  |
| Magnetic sensors; Magnetically assisted SERS sensors |  |
| Advanced electrochemical sensors |  |
| Graphene based nanosensors |  |
|  | |
| **WP9 TOXICITY AND RISKS OF NANOMATERIALS** | |
| Health risks |  |
| Environmental risks |  |
| „In vitro“ and „in vivo“ toxicity tests – cytotoxicity, genotoxicity, interactions with membrane |  |
| RNA gene expression changes and protein expression changes |  |
| Complete eco/aquatoxicity ecotoxicity evaluation |  |
| Toxicity against bacteria and fungi |  |

**Detailed description of expertise**

**Please, specify the main research topics connected with equipment**:

Computer simulations of complex molecular systems at atomistic level (Molecular dynamics, QM) with main focus to dendrimers, in the framework of research of their biomedical applications.

**Please, specify the secondary research topics connected with equipment**:

**Keywords describing research area:**

Computer simulations

**Competence**

**Relevance for applied and industrial research:**

**Relevance for fundamental studies:**

**Comments**