Yurii Ovcharenko, Ph.D.

Senior Researcher | Computational & Nuclear Materials Physics
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Nationality: Ukrainian
Current affiliation: Institute of Applied Physics, National Academy of Sciences of Ukraine

Research Profile

Senior researcher with over 20 years of experience in computational solid-state physics and multiscale modeling of radiation effects in nuclear and structural materials. Specialized in molecular dynamics simulations of defect formation, cascade processes, and microstructure evolution in zirconium-based alloys and nuclear fuel materials. Extensive long-term experience in international collaboration with Chinese research institutes, including projects conducted in **Chengdu (Sichuan Province)**. Author of more than 50 scientific publications in peer-reviewed international journals.

Research Interests

- Molecular dynamics simulations of radiation damage

- Multiscale and multilevel modeling of defect evolution

- Nuclear materials and zirconium-based alloys

- Radiation-induced cascades and defect clustering

- Phase-field and continuum modeling of microstructure

- Interaction of radiation defects with dislocations and grain boundaries

- X-ray interaction with materials and phase-contrast imaging

- Scientific data analysis and high-performance computing

Materials Properties Expertise

- Radiation-induced defect formation energies and migration barriers

- Diffusion coefficients of point defects and impurity atoms (O, H, Xe)

- Stress–strain behavior and elastic properties of irradiated materials

- Cascade damage morphology and defect cluster size distributions

- Radiation-induced swelling and microstructural stability

- Thermal annealing and recovery behavior of radiation damage

- Adsorption energies and surface diffusion mechanisms on metals and oxides

- Grain re-orientation and grain boundary interaction with defects

- Optical and X-ray properties of metals and alloys under mechanical deformation

Education

Ph.D. in Solid State Physics (1999)
Sumy State University, Ukraine

M.Sc. (Specialist Degree) in Physics, Mathematics and Computer Science (1993)
Sumy State Pedagogical Institute, Ukraine
Qualification: Teacher of Physics and Computer Science

Academic and Professional Positions

Senior Researcher (2015 – present)
Institute of Applied Physics, National Academy of Sciences of Ukraine - Department

of Modelling of Radiation Effects and Microstructure Transformations in Structural Materials (2015–2024) - Laboratory of X-ray Phase-Contrast Tomography Based on Compact Accelerators (2025–present)

Associate Professor (2002–2013)
Department of General and Theoretical Physics, Sumy State University

Senior Lecturer / Assistant Professor (1998–2002)
Department of Theoretical Physics, Sumy State University

International Research Collaboration (China)

Long-term collaboration with Chinese academic and industrial research organizations, including institutes located in **Chengdu, Sichuan Province**.

Selected joint research projects: - *Multiscale modeling of radiation defect dynamics and vacancy cluster formation in pure zirconium* (2016) - *Radiation defects in binary and ternary Zr–Sn–Nb alloy systems* (2018–2019) - *Interaction of dislocations, grain boundaries and radiation defects in neutron-irradiated zirconium alloys* (2019–2020) - *Mechanical properties and microstructural evolution of U_3Si_2 under interaction with fission gases* (2021)

Contract researcher at **NPIC (China)**: 2021–2024

Research Projects and Grants

- **Project Leader**: *Integrated modeling and nuclear-physical methods for studying radiation damage in materials under irradiation* (2025–2026)
- Responsible executor of national research projects on multiscale modeling of radiation damage and defect self-organization (2016–2021)

Academic Supervision

- Official **Ph.D. supervisor of two doctoral (Ph.D.) students** in physics/materials science

- Experience in mentoring graduate students and young researchers in computational physics, molecular dynamics, and advanced data analysis

Advanced Computational Expertise

Advanced development of **custom computational frameworks** for non-standard physical problems that cannot be efficiently solved using off-the-shelf molecular dynamics or post-processing tools.

- Design and implementation of **automated scientific workflows**: programs that generate, compile, configure and execute other simulation codes for large-scale computational studies of physical processes in materials
- Advanced **post-processing of large simulation datasets** (tens of GB per file) for extraction of physical observables, construction of graphical dependencies, and quantitative analysis of results
- **Symbolic and analytical computation**: programmatic differentiation of complex analytical expressions; automated generation of large systems of algebraic equations (thousands of terms per equation) involving rational expressions with unknowns in both numerators and denominators at different powers
- Development and application of **high-precision numerical solvers** for large nonlinear algebraic systems with user-defined accuracy
- Design of **multithreaded analysis codes** for efficient processing of large LAMMPS dump files, enabling specialized analyses beyond standard LAMMPS or OVITO capabilities (e.g. diffusion processes under surface physical adsorption and variable-particle-number conditions where conventional MSD methods are not applicable)
- Development of **error-robust and reproducible computational pipelines**, significantly reducing manual intervention and minimizing the risk of accidental errors in large computational projects

X-ray and Optical Modeling Expertise

- Modeling of **X-ray diffraction and scattering** on structural inhomogeneities in crystalline and polycrystalline materials
- Use of **molecular dynamics and ab initio simulation results** for calculation of optical and scattering characteristics of materials in the X-ray range
- Application of computational modeling to problems in **X-ray defectoscopy, phase-contrast tomography, and development of X-ray instrumentation**
- Strong orientation toward both **fundamental research and applied/industrial tasks** related to X-ray technologies

Teaching Experience

- Extensive university-level teaching experience in theoretical physics and computational materials science
- **Developer of a specialized graduate-level course**: *"Molecular Dynamics and ab initio Modeling in Materials Science"* (2025)
- Experience in integrating modern computational methods into physics and materials science education

Technical Skills

Simulation & Modeling
- Molecular Dynamics (MD) - Multiscale and multilevel modeling - Phase-field modeling

Programming & Data Analysis
- Python, MATLAB, Perl, PHP
- High-performance and multithreaded data analysis - Scientific data parsing, filtering and analysis

Databases & Version Control
- MySQL, SQLite
- Git, SVN

Operating Systems
- Linux / Unix

Selected Publications (International Journals)

1. Rongjian Pan et al., **Ovcharenko Y.M.**, *Microstructure evolution of cascade annealing in irradiated α-Zr*, Radiation Effects and Defects in Solids, 2019.
2. Z. Wang et al., **Ovcharenko Y.M.**, *Stress-driven grain re-orientation and merging behaviour in zirconium alloy oxidation*, Corrosion Science, 2019.
3. Rongjian Pan et al., **Ovcharenko Y.M.**, *Unveiling the feature of deposition of oxygen and water molecules on the zirconium surface*, Materials Today Communications, 2024.

4. Rongjian Pan et al., **Ovcharenko Y.M.**, *Adsorption and diffusion of oxygen atoms on Zr and ZrO_2 crystals with point defects*, Journal of Nuclear Materials, 2024.
5. Kokhan S.V. et al., **Ovcharenko Y.M.**, *Atomic displacements produced in cascades in irradiated α-Zr by molecular dynamics simulations*, Metallofizika i Noveishie Tekhnologii, 2016.

(Full publication list available upon request or via Google Scholar)

Academic Honors

- Diploma of the Presidium of the National Academy of Sciences of Ukraine for contributions to solid-state physics and materials science (two awards)

Languages

- Ukrainian – native
- Russian – native
- English – working proficiency (scientific and professional communication)

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