

# Petr Grigorev | Computational Physicist

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## Education

<b>Ghent University/Complutense University of Madrid</b> <i>Ph.D. in Engineering Physics</i> International Doctoral College in Fusion Science and Engineering (FUSION-DC)	<b>Ghent/Madrid</b> 2012–2017
<b>Peter the Great St.Petersburg Polytechnic University</b> <i>Master in Physics, GPA 5.0 out of 5.0</i> Specialization in Nuclear and Elementary Particle Physics	<b>Saint-Petersburg</b> 2010–2012
<b>Peter the Great St.Petersburg Polytechnic University</b> <i>Bachelor in Physics, GPA 4.4 out of 5.0</i> Department of Nuclear Physics	<b>Saint-Petersburg</b> 2006–2010

## Ph.D. thesis

**title:** *Assessment of retention of plasma components in tungsten under high flux plasma exposure: multi-scale modelling approach*

**supervisors:** Dr. Dmitry Terentyev, Dr. Christophe Ortiz

**date of the defence:** 27 April 2017

**description:** A new physical model of dislocation mediated H retention in tungsten under fusion relevant plasma exposure conditions was proposed. A Rate Theory simulation tool was developed and validated by comparison with experimental results available in literature.

## Master thesis

**title:** *Molecular dynamics study of sputtering of Al, Si and SiC surfaces and nanoclusters by monoatomic and nanocluster beams*

**supervisor:** Dr. Evgeny E. Zhurkin

## Experience

Research.....

<b>Centre Interdisciplinaire de Nanoscience de Marseille</b> <i>Post-Doctoral researcher</i> Project title: <i>Mesoscale models from massively parallel atomistic simulations: uncertainty driven, self-optimizing strategies for hard materials</i> Research tasks: <ul style="list-style-type: none"><li>○ Setting up and performing massively paralleled Molecular Dynamics simulations;</li><li>○ Data analysis, coarse graining and uncertainty quantification;</li><li>○ Dissemination of the results and search of possible applications of the developed tool set;</li></ul>	<b>Marseilles</b> 2020–present
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**Warwick Centre for Predictive Modelling****Coventry***Research Fellow**2017–2020*

Development and application of a set of atomistic materials modelling methods:

- Hybrid quantum/classical methods to study dislocations and cracks in metals and semiconductors;
- Classical and machine learning based force fields;
- Uncertainty quantification in atomistic models as well as uncertainty propagation in upper scale models;

**Belgian Nuclear Research Centre SCK•CEN in collaboration with CIEMAT Mol/Madrid***Ph.D. student**2012–2017***Belgian Nuclear Research Centre SCK•CEN****Mol***Internship**2012*

Study of radiation hardening of high-Cr steels and model Fe-Cr alloys due to dislocation loops. Results of a large number of MD simulations were analysed in order to provide an input for Dislocation Dynamics (DD) simulation tool.

**Scientific and Educational Centre "Hadron"****Saint-Petersburg***Assistant researcher**2010–2012*

Performing research tasks for the master thesis.

**Petersburg Nuclear Physics Institute****Gatchina***Bachelor thesis internship**2010*

The internship was done in the laboratory of nuclear and elementary particles physics. During the internship VITESS simulation package was modified and used in order to study the possibility of obtaining monochromatic neutron beams from a fission neutron beam.

**Invited presentations.....****Computational Materials Science Seminar****Skoltech Moscow***Multiscale QM/MM modelling of materials chemomechanics**10th October 2019***Seminar of Service de Recherche en Métallurgie Physique****CEA Paris-Saclay***QM/MM study of hydrogen decorated screw dislocations in tungsten**17th June 2019***Awards.....**

Warwick Faculty of Science, Engineering and Medicine Post-doctoral Research Prize 2020

**Service to profession.....****Reviewer for:** Journal of Nuclear Materials, Scripta Materialia, Philosophical Magazine**Contribution to open-source software:** libAtoms/matscipy, Atomic Simulation Environment**Computer skills****Languages:** Fortran, C/C++, Python**Simulation packages:** LAMMPS, VASP, ASE**Operating Systems:** Windows, Linux, MacOS**SciPy:** NumPy, matplotlib, pandas, bokeh**MS Office:** Word, PowerPoint, Excel**Other:** L<sup>A</sup>T<sub>E</sub>X, Git, Jupyter notebooks**Languages****Russian:** Mother tongue**English:** C1 CEFR level (academic IELTS 7.5)**Italian:** A1 CEFR level**French:** A1 CEFR level**Interests****Sports:** Football, Snowboarding, Swimming, Running**Other:** Hiking, Graphic art, Data visualisation