

# Igor Poltavsky

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| CONTACT INFORMATION | Senior Researcher<br>University of Luxembourg,<br>Campus Limpertsberg,<br>162A Avenue de la Faïencerie,<br>L-1511, Luxembourg   | <i>E-mail:</i> igor.poltavskyi@uni.lu |
| RESEARCH INTERESTS  | Statistical physics, imaginary-time path integral methods, nuclear quantum effects, <i>ab initio</i> simulations  |                                       |
| WORKING EXPERIENCE  | <i>Senior Researcher</i><br>University of Luxembourg, 162A Avenue de la Faïencerie, L-1511 Luxembourg   | <b>January, 2016 - present</b>        |
|                     | <i>Postdoctoral Fellow</i><br>Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany  | <b>December, 2013 - January, 2016</b> |
|                     | <i>Postdoctoral Fellow</i><br>Institute of Theoretical and Computational Chemistry at POSTECH, San 31 Hyojadong, Namgu, Pohang, Kyungbuk 790-784, Korea   | <b>July, 2012 - December, 2013</b>    |
|                     | <i>Junior Research Associate</i><br>B. Verkin Institute for Low Temperature Physics & Engineering, National Academy of Sciences of Ukraine, 47 Lenin Ave., Kharkov, 61164, Ukraine  | <b>April, 2009 - July, 2012</b>       |
| EDUCATION           | <b>B. Verkin Institute for Low Temperature Physics &amp; Engineering</b> , Kharkov, Ukraine<br>Ph.D. in Theoretical Physics, April, 2009<br>Dissertation Topic: “Structural, thermal and magnetic properties of atomic and molecular cryocrystals.”   |                                       |
|                     | <b>Kharkiv State University</b> , Kharkiv, Ukraine<br>M.S., Radiophysics and Electronics, July, 2003  |                                       |
|                     | <b>Kharkiv State University</b> , Kharkiv, Ukraine<br>B.A., Theoretical Radiophysics, June, 2002  |                                       |
| HONORS AND AWARDS   | The grant for young scientists of the National Academy of Sciences of Ukraine, 2009-2011  |                                       |
| COMPUTER SKILLS     | <ul style="list-style-type: none"><li>• Languages: Python, Fortran, C++, Mathematica, some use of Unix shell scripts, MPI parallel processing library.</li><li>• Tools and Packages: FHI-aims, i-Pi, OpenMM, L<sup>A</sup>T<sub>E</sub>X, MS Office, and presentation software.</li><li>• Operating Systems: OS X, Unix/Linux, Windows.</li></ul> |                                       |
| LANGUAGES           | English, Russian, Ukrainian   |                                       |

## PUBLICATIONS

1. T. N. Antsygina, K. A. Chishko, I. A. Degtyaryov, I. Poltavsky, S. S. Sokolov, N. Studart, Plasma excitation dispersion in non-degenerate quantum wire over liquid helium, *Eur. Phys. J. B* **90**, P. 79 (2017).
2. S. Chmiela, A. Tkatchenko, H.E. Sauceda, I. Poltavsky, K. T. Schütt, and K.-R. Müller, Machine learning of accurate energy-conserving molecular force fields, *Sc. Adv.* **3** (2017).
3. M. Chattopadhyaya, J. Hermann, I. Poltavsky, and A. Tkatchenko, Tuning intermolecular interactions with nanostructured environments, *Chem. Mater.* **29**, P. 2452 (2016).
4. I. Poltavsky, L. Zheng, M. Mortazavi, and A. Tkatchenko, Quantum Tunneling of Thermal Protons Through Pristine Graphene, arXiv:1605.06341v2 (2016).
5. R. J. Maurer, W. Liu, I. Poltavsky, T. Stecher, H. Oberhofer, K. Reuter, and A. Tkatchenko, Thermal and electronic fluctuations of flexible adsorbed molecules: Azobenzene on Ag (111), *Phys. Rev. Lett.* **116**, 146101 (2016).
6. I. Poltavsky and A. Tkatchenko, Modeling quantum nuclei with perturbed path integral molecular dynamics, *Chem. Sci.* **7**, P. 1368 (2016).
7. I. I. Poltavsky, T. N. Antsygina, M. I. Poltavskaya, and K. A. Chishko, Magnetization of 3 He layers in ferromagnetic regime: Cluster size effects, *Physica B: Condensed Matter* **407** (19), P. 3925 (2012).
8. T. N. Antsygina, M. I. Poltavskaya, I. I. Poltavsky, and K. A. Chishko, Excitation spectra of hard-core bosons on square and triangular lattices in superfluid phase, *Phys. Rev. B* **82**, P. 144504 (2010).
9. T. N. Antsygina, M. I. Poltavskaya, I. I. Poltavsky, and K. A. Chishko, Square lattice hard-core bosons within the random phase approximation, *Phys. Rev. B* **80**, P. 174511 (2009).
10. T. N. Antsygina, I. I. Poltavsky, M. I. Poltavskaya, and K. A. Chishko, Thermodynamics of low-dimensional spin-1/2 Heisenberg ferromagnets in an external magnetic field within Green function formalism, *Phys. Rev. B* **77**, P. 024407 (2008).
11. T. N. Antsygina, I. I. Poltavsky, M. I. Poltavskaya, and K. A. Chishko, Heat capacity and spin susceptibility of two-dimensional t-J model, *Fizika Nizkikh Temperatur* **33**, P. 814 (2007).
12. T. N. Antsygina, I. I. Poltavsky, and K. A. Chishko, Exactly solved model for 4 He adsorption on carbon nanotube bundles, *J. Low Temp. Phys.* **148**, P. 821 (2007).
13. T. N. Antsygina, I. I. Poltavsky, and K. A. Chishko, Thermodynamics of low-dimensional adsorption in grooves, on the outer surface, and in interstitials of a close-ended carbone nanotube bundle, *Phys. Rev. B* **74**, P. 205429 (2006).
14. T. N. Antsygina, I. I. Poltavsky, K. A. Chishko, T. A. Wilson and O. E. Vilches, Thermodynamics of quasi-one-dimensional deposits on carbon nanobundles, *Fizika Nizkikh Temperatur* **31**, P. 1328 (2005).
15. T. N. Antsygina, I. I. Poltavsky, and K. A. Chishko. Dynamics and thermodynamics of quasi-one-dimensional helium deposited on carbon nano-bundles, *J. Low Temp. Phys.* **138**, P. 223 (2005).
16. T. N. Antsygina, I. I. Poltavsky, M. I. Poltavskaya, and K. A. Chishko, Lattice dynamics and heat capacity of a two-dimensional monoatomic crystal on a substrate, *Fizika Nizkikh Temperatur* **28**, P. 621 (2002).
17. T. N. Antsygina, I. I. Poltavsky, and K. A. Chishko, Lattice dynamics of 2D monoatomic crystal: Application to 3 He on graphite, *J. Low Temp. Phys.* **126**, P. 15 (2002).

\* In my first ten articles the alphabetical ordering in Cyrillic alphabet has been used. This ordering was common in former Soviet Union and often does not reflect real contribution to the paper.