IVAN I. OLEYNIK
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Education

Russian Academy of Sciences, Moscow	Chemical Physics	Ph.D.	1992
Moscow Institute of Physics and Technology	Physics	M.Sc.	1983

Appointments

- Professor, Associate Professor, Assistant Professor, Department of Physics, University of South Florida, 2002-present
- Director, NSF REU Site in Applied Physics at the University of South Florida, 2010-2014
- Research Scientist, Senior Research Scientist, Department of Materials, University of Oxford, UK, 1996-2001
- The Royal Society Research Fellow, School of Physics, University of Bath, UK, 1995-1996
- Assistant Professor, Department of Applied Mathematics, Volgograd State University, Russia, 1992-1995
- Research Assistant, Russian Academy of Sciences, Institute of Chemical Physics, Moscow, Russia, 1988-1992

Honors, Awards and Fellowships

- APS Fellow, 2015
- USF Outstanding Research Award, 2012
- ONR/NRL Summer Faculty Fellowship, 2003-2005
- The Royal Society Research Fellowship, 1995-1996
- AFOSR/EOARD Window on Science (WOS) award, 1993

Professional service

- Chair of 2015 APS International Conference “Shock Compression of Condensed Matter”
- Organizer of focus sessions “Materials in Extremes: Bridging Simulation and Experiment”, at APS 2012-2017 March Meetings
- Chair of “2D Materials” Focus Topic at American Vacuum Society International Symposia (2010-2017)
- Chair of USF System Research Council; member of USF Faculty Senate Executive Committee (2015-2016); member of USF System Research Council (2012-2016)

Research interests

- Computer-aided discovery of new materials with unique electronic, vibrational, thermal, mechanical, optical, transport and superconducting properties
- Simulation of matter at extreme conditions of high pressure, high temperature and high strain rates
- Novel high-nitrogen content energetic materials, superhard materials, 2D materials for energy applications
- Development of interatomic potentials for large-scale simulations of materials
- Charge, spin and thermal transport in single molecules and magnetic tunnel junctions

Selected publications

1 J. M. Gonzalez and I. I. Oleynik, "Layer-dependent Properties of SnS_2 And $SnSe_2$ Two-dimensional Materials", *Phys. Rev. B.* **94**, 1 (2016) http://dx.doi.org/10.1103/PhysRevB.94.125443

2 B. A. Steele and I. I. Oleynik, "Sodium Pentazolate: A Nitrogen Rich High Energy Density Material", *Chem. Phys. Lett.* **643**, 21 (2016) http://dx.doi.org/10.1016/j.cplett.2015.11.008

3 B. A. Steele and I. I. Oleynik, "New Phase of Ammonium Nitrate: A Monoclinic Distortion of AN-IV", *J. Chem. Phys.* **143**, 234705 (2015) http://dx.doi.org/10.1063/1.4937420

4 M. A. Kozhushner, B. V. Lidskii, I. I. Oleynik, V. S. Posvyanskii, and L. I. Trakhtenberg, "Inhomogeneous Charge Distribution in Semiconductor Nanoparticles", *J. Phys. Chem. C* **119**, 16286 (2015) http://dx.doi.org/10.1021/acs.jpcc.5b01410

5 V. V. Zhakhovsky, M. M. Budzevich, A. C. Landerville, I. I. Oleynik, and C. T. White, "Laminar, Cellular, Transverse, and Multiheaded Pulsating Detonations in Condensed Phase Energetic Materials From Molecular Dynamics Simulations", *Phys. Rev. E* **90**, 33312 (2014) http://dx.doi.org/10.1103/PhysRevE.90.033312

6 J. C. Crowhurst, J. M. Zaug, H. B. Radousky, B. A. Steele, A. C. Landerville, and I. I. Oleynik, "Ammonium Azide Under High Pressure: A Combined Theoretical and Experimental Study", *J. Phys. Chem. A* **118**, 8695 (2014) http://dx.doi.org/10.1021/jp502619n

7 B. J. Demaske, V. V. Zhakhovsky, N. A. Inogamov, and I. I. Oleynik, "Ultrashort Shock Waves in Nickel Induced by Femtosecond Laser Pulses", *Phys. Rev. B* **87**, 54109 (2013) http://dx.doi.org/10.1103/PhysRevB.87.054109

8 M. A. Kozhushner, L. I. Trakhtenberg, A. C. Landerville, and I. I. Oleynik, "Theory of Sensing Response of Nanostructured Tin-Dioxide Thin Films To Reducing Hydrogen Gas", *J. Phys. Chem. C* **117**, 11562 (2013) http://dx.doi.org/10.1021/jp311847j

9 R. Perriot, X. Gu, Y. Lin, V. V. Zhakhovsky, and I. I. Oleynik, "Screened Environment-dependent Reactive Empirical Bond-order Potential For Atomistic Simulations of Carbon Materials", *Phys. Rev. B* **88**, 64101 (2013) http://dx.doi.org/10.1103/PhysRevB.88.064101

10 L. Adamska, R. Addou, M. Batzill, and I. I. Oleynik, "Atomic and Electronic Structure of Graphene/Sn-Ni(111) and Graphene/Sn-Cu(111) Surface Alloy Interfaces", *Appl. Phys. Lett.* **101**, 51602 (2012) http://dx.doi.org/10.1063/1.4739475

11 L. Adamska, Y. Lin, A. J. Ross, M. Batzill, and I. I. Oleynik, "Atomic and Electronic Structure of Simple Metal/graphene and Complex Metal/graphene/metal Interfaces", *Phys. Rev. B* **85**, 195443 (2012) http://dx.doi.org/10.1103/PhysRevB.85.195443

12 M. M. Budzevich, V. V. Zhakhovsky, C. T. White, and I. I. Oleynik, "Evolution of Shock-Induced Orientation-Dependent Metastable States in Crystalline Aluminum", *Phys. Rev. Lett.* **109**, 125505 (2012) http://dx.doi.org/10.1103/PhysRevLett.109.125505

13 V. V. Zhakhovsky, M. M. Budzevich, N. A. Inogamov, I. I. Oleynik, and C. T. White, "Two-Zone Elastic-Plastic Single Shock Waves In Solids", *Phys. Rev. Lett.* **107**, 135502 (2011) http://dx.doi.org/10.1103/PhysRevLett.107.135502

14 J. Lahiri, T. Miller, L. Adamska, I. I. Oleynik, and M. Batzill, "Graphene Growth on Ni(111) by Transformation of A Surface Carbide.", *Nano Lett.* **11**, 518 (2011) http://dx.doi.org/10.1021/nl103383b

15 J. Lahiri, T. S Miller, A. J Ross, L. Adamska, I. I. Oleynik, and M. Batzill, "Graphene Growth and Stability at Nickel Surfaces", *New J. Phys.* **13**, 25001 (2011) http://dx.doi.org/10.1088/1367-2630/13/2/025001

16 L. Adamska, M. A. Kozhushner, and I. I. Oleynik, "Electron-plasmon Interactions in Resonant Molecular Tunnel Junctions", *Phys. Rev. B* **81**, 35404 (2010) http://dx.doi.org/10.1103/PhysRevB.81.035404

17 J. Lahiri, Y. Lin, P. Bozkurt, I. I. Oleynik, and M. Batzill, "An Extended Defect in Graphene As A Metallic Wire.", *Nat. Nanotechnol.* **5**, 326 (2010) http://dx.doi.org/10.1038/nnano.2010.53

18 A. C. Landerville, M. W. Conroy, M. M. Budzevich, Y. Lin, C. T. White, and I. I. Oleynik, "Equations of State For Energetic Materials From Density Functional Theory with van Der Waals, Thermal, and Zero-point Energy Corrections", *Appl. Phys. Lett.* **97**, 251908 (2010) http://dx.doi.org/10.1063/1.3526754

19 B. J. Demaske, V. V. Zhakhovsky, N. A. Inogamov, and I. I. Oleynik, "Ablation and Spallation of Gold Films Irradiated by Ultrashort Laser Pulse", *Phys. Rev. B* **82**, 64113 (2010) http://dx.doi.org/10.1103/PhysRevB.82.064113

20 J. Hihath, Y. Lee, L. Yu, L. Adamska, M. A. Kozhushner, I. I. Oleynik, and N. Tao, "Rectification and Stability of A Single Molecular Diode with Controlled Orientation.", *Nat. Chem.* **1**, 635 (2009) http://dx.doi.org/10.1038/nchem.392

21 M. W. Conroy, I. I. Oleynik, S. V Zybin, and C. T. White, "Density Functional Theory Calculations of Solid Nitromethane Under Hydrostatic and Uniaxial Compressions with Empirical van Der Waals Correction.", *J. Phys. Chem. A* **113**, 3610 (2009) http://dx.doi.org/10.1021/jp809843k

22 A. C. Landerville, I. I. Oleynik, and C. T. White, "Reactive Molecular Dynamics of Hypervelocity Collisions of PETN Molecules.", *J. Phys. Chem. A* **113**, 12094 (2009) http://dx.doi.org/10.1021/jp905969y

23 M. Conroy, I. Oleynik, S. Zybin, and C. White, "First-principles Investigation of Anisotropic Constitutive Relationships in Pentaerythritol Tetranitrate", *Phys. Rev. B* **77**, 94107 (2008) http://dx.doi.org/10.1103/PhysRevB.77.094107

24 M. W. Conroy, I. I. Oleynik, S. V. Zybin, and C. T. White, "Density Functional Theory Calculations of Anisotropic Constitutive Relationships in Alpha-cyclotrimethylenetrinitramine", *J. Appl. Phys.* **104**, 113501 (2008) http://dx.doi.org/10.1063/1.2973689

25 J. E. Butler and I. I. Oleynik, "A Mechanism For Crystal Twinning in The Growth of Diamond by Chemical Vapour Deposition.", *Philos. Trans. A. Math. Phys. Eng. Sci.* **366**, 295 (2008) http://dx.doi.org/10.1098/rsta.2007.2152

26 E. Y. Tsymbal, K. D. Belashchenko, J. Velev, S. S. Jaswal, M. Vanschilfgaarde, I. I. Oleynik, and D. A. Stewart, "Interface Effects in Spin-dependent Tunneling", *Prog. Mater. Sci.* **52**, 401 (2007) http://dx.doi.org/10.1016/j.pmatsci.2006.10.009

27 I. I. Oleynik, M. A. Kozhushner, V. S. Posvyanskii, and L. Yu, "Rectification Mechanism in Diblock Oligomer Molecular Diodes", *Phys. Rev. Lett.* **96**, 96803 (2006) http://dx.doi.org/10.1103/PhysRevLett.96.096803

28 M. A. Kozhushner, V. S. Posvyanskii, and I. I. Oleynik, "Bound States of Tunneling Electrons in Molecular Chains", *Phys. Rev. B* **74**, 165103 (2006) http://dx.doi.org/10.1103/PhysRevB.74.165103

29 M. A. Kozhushner, V. S. Posvyanskii, and I. I. Oleynik, "Tunneling and Resonant Conductance in One-dimensional Molecular Structures", *Chem. Phys.* **319**, 368 (2005) http://dx.doi.org/10.1016/j.chemphys.2005.06.023

30 D. G. Pettifor and I. I. Oleynik, "Interatomic Bond-order Potentials and Structural Prediction", *Prog. Mater. Sci.* **49**, 285 (2004) http://dx.doi.org/10.1016/S0079-6425(03)00024-0

31 I. I. Oleynik and E. Y. Tsymbal, "Metal-Oxide Interfaces in Magnetic Tunnel Junctions", *Interface Sci.* **12**, 105 (2004) http://dx.doi.org/10.1023/B:INTS.0000012299.56792.ae

32 K. Belashchenko, E. Tsymbal, M. van Schilfgaarde, D. Stewart, I. Oleynik, and S. Jaswal, "Effect of Interface Bonding on Spin-dependent Tunneling From The Oxidized Co Surface", *Phys. Rev. B* **69**, 174408 (2004) http://dx.doi.org/10.1103/PhysRevB.69.174408

33 D. G. Pettifor and I. I. Oleynik, "Interatomic Bond-order Potentials and Structural Prediction", *Prog. Mater. Sci.* **49**, 285 (2004) http://dx.doi.org/10.1016/S0079-6425(03)00024-0

34 I. I. Oleynik and E. Y. Tsymbal, "Atomic, Electronic, and Magnetic Properties of Magnetic Tunnel Junctions", *J. Appl. Phys.* **93**, 6429 (2003) http://dx.doi.org/10.1063/1.1558631

35 D. Pettifor and I. Oleinik, "Analytic Bond-order Potential For Open and Close-packed Phases", *Phys. Rev. B* **65**, 172103 (2002) http://dx.doi.org/10.1103/PhysRevB.65.172103

36 D. G. Pettifor, I. I. Oleinik, D. Nguyen-Manh, and V. Vitek, "Bond-order Potentials: Bridging The Electronic To Atomistic Modelling Hierarchies", *Comput. Mater. Sci.* **23**, 33 (2002) http://dx.doi.org/10.1016/S0927-0256(01)00204-X

37 I. I. Oleinik, E. Y. Tsymbal, and D. G. Pettifor, "Atomic and Electronic Structure of Co/SrTiO3/Co Magnetic Tunnel Junctions", *Phys. Rev. B* **65**, 20401 (2001) http://dx.doi.org/10.1103/PhysRevB.65.020401

38 I. I. Oleinik, E. Y. Tsymbal, and D. G. Pettifor, "Structural and Electronic Properties of Co/Al2O3/Co Magnetic Tunnel Junction From First Principles", *Phys. Rev. B* **62**, 3952 (2000) http://dx.doi.org/10.1103/PhysRevB.62.3952

39 I. I. Oleinik, D. G. Pettifor, A. P. Sutton, and J. E. Butler, "Theoretical Study of Chemical Reactions on CVD Diamond Surfaces", *Diam. Relat. Mater.* **9**, 241 (2000) http://dx.doi.org/10.1016/S0925-9635(99)00312-X

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42 I. I. Oleinik and D. G. Pettifor, "Analytic Bond-order Potentials Beyond Tersoff-Brenner. II. Application To The Hydrocarbons", *Phys. Rev. B* **59**, 8500 (1999) http://dx.doi.org/10.1103/PhysRevB.59.8500

43 C. C. Battaile, D. J. Srolovitz, I. I. Oleinik, D. G. Pettifor, A. P. Sutton, S. J. Harris, and J. E. Butler, "Etching Effects During The Chemical Vapor Deposition of (100) Diamond", *J. Chem. Phys.* **111**, 4291 (1999)