PIERRE DARANCET

Assistant Scientist

Theory and Modeling Group

Center for Nanoscale Materials
Building 440, Room A235
Phone: 630-252-4709
Fax: 630-252-4646
E-mail: pdarancet@anl.gov

Argonne National Laboratory
9700 S Cass Ave., Argonne, IL 60439

Education

Ph.D., Physics, Université Joseph Fourier, Grenoble	2008
M.Sc. Applied Physics, Institut National des Sciences Appliquées, Toulouse	2005
M.Sc. Physics, Université Paul Sabatier, Toulouse	2005

Awards and honors

Ph.D. Fellowship, French Ministry of Education, Research and Technology (MENRT)	2005-2008
Graduated with Honors, first class. University Paul Sabatier, Toulouse	2005

Research interests

- Modeling non-equilibrium charge and energy transport using first-principles methods
- Optoelectronic properties of nanomaterials and heterogeneous interfaces
- Novel methods for electron and exciton dynamics accounting for many-body interactions
- Wave-like charge and energy transport in mesoscale devices
- Current- and bias-driven structural evolution

Professional Experience

Argonne National Laboratory - Center for Nanoscale Materials (CNM) — 2014-present
Assistant Scientist

Northwestern Argonne Institute for Science and Engineering (NAISE) — 2016-present
Institute Fellow

Columbia University, Departments of Physics and Applied Physics — 2012-2014
Postdoctoral Research Scientist

Lawrence Berkeley National Lab., Molecular Foundry — 2008-2012
Postdoctoral Fellow

Institut Néel, CNRS/UJF — 2005-2008
Research Assistant

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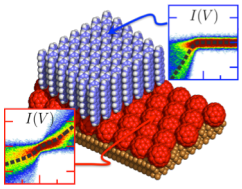
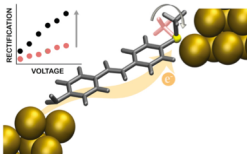
Selected Publications

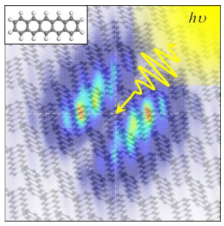
First-principles modeling of charge and energy transport



1. Large Spatially Resolved Rectification in a Donor–Acceptor Molecular Heterojunction, J. A. Smerdon, N. C. Giebink, N. P. Guisinger, **P. Darancet,** J. R. Guest*, Nano Letters* **16** *(4), 2603-2607* (2016).

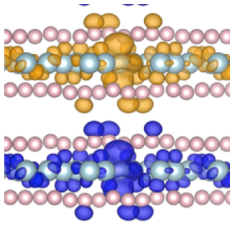


2. Determination of Energy Level Alignment and Coupling Strength in 4,4'-Bipyridine Single-Molecule Junctions, T. Kim, **P. Darancet**, J. R. Widawsky, M. Kotiuga, S. Y. Quek, J. B. Neaton, L. Venkataraman, *Nano Letters,* **14** *(2), 794-798* (2014).



3. Tuning rectification in Highly Conductive Single-Molecular Diodes, A. Batra, **P. Darancet**, Q. Chen, J. S. Meisner, J. R. Widawsky, J. B. Neaton, C. V. Nuckolls, L. Venkataraman*, Nano Letters,* **13** *(12), 6233-6237* (2013).
4. Low-Energy Charge-Transfer Excitons in Organic Solids from First-Principles: The Case of Pentacene, S. Sharifzadeh, **P. Darancet**, L. Kronik, J. B. Neaton, *The Journal of Physical Chemistry Letters,* **4** *(13), 2197-2201* (2013).

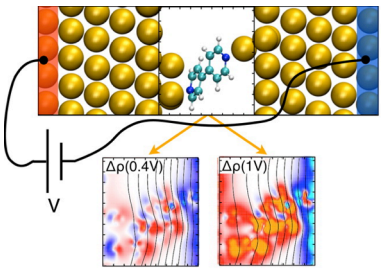
Electronic Structure of nanomaterials and interfaces



5. Three-dimensional metallic and two-dimensional insulating behavior in octahedral tantalum dichalcogenides, **P. Darancet**, A. J. Millis, C. A. Marianetti, *Physical Review B,* **90** *(4), 045134* (2014).
6. Physical Adsorption and Charge Transfer of Molecular Br2 on Graphene, Z. Chen, **P. Darancet**, L. Wang, A. C. Crowther, Y. Gao, C. R. Dean, T. Taniguchi, K. Watanabe, J. Hone, C. A. Marianetti, L. E. Brus, *ACS Nano* **8** *(3), 2943-2950* (2014).
7. Electronic Energy Level Alignment at Metal-Molecule Interfaces with a GW Approach, I. Tamblyn, **P. Darancet**, S. Y. Quek, S. A. Bonev, J. B. Neaton, *Physical Review B,* **84***, 201402* (2011).

Theoretical predictions

8. Adsorption-Induced Solvent-Based Electrostatic Gating of Charge Transport through Molecular Junctions, M. Kotiuga**, P. Darancet**, C. R. Arroyo, L. Venkataraman, J. B. Neaton, *Nano Letters,* **15** *(7), 4498-4503* (2015).
9. Coherent Electronic Transport through Graphene Constrictions: Subwavelength Regime and Optical Analogy, **P. Darancet**, V. Olevano, D. Mayou, *Physical Review Letters,* **102,** *136803* (2009).



Method development

10. Quantitative Current-Voltage Characteristics in Molecular Junctions from First Principles, **P. Darancet**, J. R. Widawsky, H. J. Choi, L. Venkataraman, J. B. Neaton, *Nano Letters,* **12***, 6250-6254* (2012).
11. Quantum Transport through Resistive Nanocontacts: Effective One-dimensional Theory and Conductance Formulas for Nonballistic Leads, **P. Darancet**, V. Olevano, D. Mayou, *Physical Review B,* **81,** *155422* (2010).