



Dr. David Dell'Angelo

CONTACT INFORMATION

Postdoctoral Researcher
Life Sciences & Engineering Center
New Jersey Institute of Technology
Newark, NJ 07102 USA

E-mail:

RESEARCH INTERESTS

Theoretical Chemical Physics & Computer Simulations: numerical implementation (theory and code development), mixed quantum-classical trajectory methods, charge and energy transfer dynamics in 2D materials, Monte Carlo methods, electronic structure calculations, quantum-mechanical effects on dynamics of nuclei, adsorption and chemisorption processes.

CURRENT ACADEMIC APPOINTMENTS

Postdoctoral Researcher

October 2020 to present

Department of Chemistry and Environmental Science , New Jersey Institute of Technology
– Code and algorithm development; models ans simulations of physical processes
– Supervisor : Assistant Professor Farnaz A. Shakib

Skills

- Quantum simulations - Density functional theory, electronic structure methods
- Material science and engineering modeling for semiconductors
- Scientific programming
- Fortran, Python, C++, Julia
- Modeling Software: Density functional theory codes (VASP, Quantum Espresso, Gaussian), Molecular Dynamics codes (LAMMPS, DL-POLY, CP2K)

RECENT WORK HISTORY

[1] Collaboration with Dr. A. Mattoni, University of Cagliari (Italy)

Research Topic:

- Development of machine learning force fields for atomistic simulations
- Application: perovskite systems, Be/C₆₀ complexes
- Methods: Gaussian Process Regression (GPR) and Neural Network (NN) methodologies, interface with molecular dynamics codes (LAMMPS) and methods for generating data training based on active learning

[2] Post-doctoral research assistant (2018-2020) University College of London (UK)

Research Topic:

- Charge and exciton reorganization energies for the system oligothiophene/fullerene (T_n/C₆₀)
- Study of charge separation at donor/acceptor heterojunctions in organic solar cells

[3] Teaching research assistant 08/2017-08/2018 University of Kumamoto (Japan)

Research Topic:

- Theoretical modeling and simulation of electronic transport in photovoltaic solar cell, with particular focus on perovskite material
- Parametrization of effective model Hamiltonians based on tight-binding approach to bridge the pictures at micro- and macro- scales in a comprehensive multi-scale simulation framework

[4] Post-doctoral research assistant 08/2015-08/2017 University of Alberta (Canada)

Research Topic:

- Implementation of transition filtering schemes for calculating observables using mixed quantum-classical Liouville surface-hopping dynamics

**REFEREED
PUBLICATIONS**

18. W.-T. Peng, D. Brey, S. Giannini, D. Dell'Angelo, I. Burghardt and J. Blumberger
Exciton Dissociation in a Model Organic Interface : Excitonic State – based Surface Hopping versus Multi – Configurational Time – Dependent Hartree
J. Phys. Chem. Lett., **13**, 7105 (2022)
17. D. Dell'Angelo, H. Ramesh, Z. Zhang, and F. A. Shakib
Architecture in the atomic microcosm : the riveting case of metal organic frameworks
In Interdisciplinarity between science and arts, 1st ed, Accepted, Springer (2022)
16. D. Dell'Angelo, M. R. Momeni and F. A. Shakib
Tuning van der Waals interactions in ultra – thin two dimensional metal – organic frameworks for photoconductive applications
Phys. Chem. Lett., Submitted (2022)
15. D. Dell'Angelo, M. R. Momeni, S. Pearson and F. A. Shakib
Modeling energy transfer and absorption spectra in layered metal – organic frameworks based on a Frenkel – Holstein Hamiltonian
J. Chem. Phys., **156**, 044109 (2022)
14. Z. Zhang, D. Dell'Angelo, M. R. Momeni, Y. Shi and F. A. Shakib
Metal – to – semiconductor transition in two – dimensional metal – organic frameworks : An ab initio dynamics perspective
ACS Appl. Mater. Interfaces, **13**, 25270 (2021)
13. M. R. Momeni, Z. Zhang, D. Dell'Angelo and F. A. Shakib
Tuning Electronic Properties of Conductive 2D Layered Metal–Organic Frameworks via Host–Guest Interactions : Dioxygen as An Electroactive Chemical Stimuli
APL Mater., **9**, 051109 (2021)
12. M. R. Momeni, Z. Zhang, D. Dell'Angelo and F. A. Shakib
Gauging van der Waals Interactions in Aqueous Solutions of 2D MOFs : When Water Likes Organic LinkersMore than Open – metal Sites
Phys. Chem. Chem. Phys., **23**, 3135 (2021)
11. D. Dell'Angelo
Computational chemistry and the study and design of catalysts
In Green Chemistry and Computational Chemistry, 1st ed, 299-332, Elsevier (2020)
10. D. Dell'Angelo, S. E. Brown, M. R. Momeni, F. A. Shakib
Downscaling an open quantum system : an atomistic approach applied to photovoltaics
In Green Chemistry and Computational Chemistry, 1st ed, 147-181, Elsevier (2020)

9. D. Dell'Angelo
Quantum Study of Helium Clusters Doped with Electronically Excited Li, Na, K and Rb Atoms
 In Advances in Quantum Systems in Chemistry, Physics, and Biology,
 Selected Proceedings of QSCP-XXIII (Kruger Park, South Africa, September 2018)
8. D. Dell'Angelo and G. Hanna
On the performance of multi – state transition filtering in mixed quantum – classical Liouville surface – hopping simulations : Beyond two – and three – state quantum Subsystems
 Theor. Chem. Acc., **15**, 137 (2018)
7. D. Dell'Angelo and G. Hanna
Importance of eigenvector sign consistency in computations of expectation values via mixed quantum – classical surface – hopping dynamics
 Theo. Chem. Acc., **136**, 75 (2017)
6. M. Li, H. Freedman, D. Dell'Angelo and G. Hanna
A model platform for rapid, robust, directed, and long-range vibrational energy transport : Insights from a mixed quantum–classical study of a 1D molecular chain
 AIP Conf. Proc., **1906**, 030007 (2017)
5. D. Dell'Angelo and G. Hanna
Using multi – state transition filtering to improve the accuracy of expectation values via mixed quantum – classical Liouville dynamics
 AIP Conf. Proc., **1790**, 020009 (2016)
4. D. Dell'Angelo and G. Hanna
Self – Consistent Filtering Scheme for Efficient Calculations of Observables via the Mixed Quantum – Classical Liouville Approach
 J. Chem. Theory Comput., **12**, 477 (2016)
3. Sophya Garashchuk, David Dell'Angelo and Vitaly Rassolov
Dynamics in the quantum/classical limit based on selective use of the quantum potential
 J. Chem. Phys., **141**, 234107 (2014)
2. David Dell'Angelo, Grégoire Guillon, and Alexandra Viel
Excited Li and Na in He_n : influence of the dimer potential energy curves
 J. Chem. Phys., **136**, 114308 (2012)
1. Michele Ceotto, David Dell'Angelo, and Gianfranco Tantardini
Multiple coherent states semiclassical initial value representation spectra calculations of lateral interactions for CO on Cu(100)
 J. Chem. Phys., **133**, 054701 (2010)

EDUCATION

Université de Rennes 1, Rennes, FRANCE

Ph.D., Physics, June 2012

- Thesis Topic: *Structure and Dynamics of Doped Helium Clusters*
- Adviser: Dr. Alexandra Viel / Professor Jean-Michel Launay

Università degli Studi di Milano, Milano, ITALY

M.S., Chemistry, October 2008

- Thesis Topic: *Classical Dynamics for the System CO adsorbed on Cu(100)*
- Adviser: Dr. Michele Ceotto / Professor Gianfranco Tantardini

LANGUAGES

- Italian : mother tongue
- English : read, written, spoken
- French : read, written, spoken
- Spanish : scolar level