Estela Blaisten-Barojas, PhD

Professor, Department of Computational and Data Sciences
Director, Center for Simulation and Modeling

Education

Doctorat d'Etat et Sciences Physiques, Paris-Sorbonne University, France

Key Interests

Nanostructures, Nanoclusters, Nanosystems | Molecular Simulation and Modeling | Soft Mater | Biomolecules | Machine Learning Applications in Condensed Matter|

CONTACT

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SELECT PUBLICATIONS

- Vortex Generation in a Finitely Extensible Nonlinear Elastic Peterkin Fluid Initially at Rest, *Engineering Reports* e12135 (2020). doi.org/10.1002eng2.12135
- Exploring with Molecular Dynamics the Structural Fate of PLGA Oligomers in Various Solvents. *Journal of Physical Chemistry B* 123, 10233 (2019).
- Simulating the NaK Eutectic Alloy with Monte Carlo and Machine Learning, *Scientific Reports 9*, 704 (2019).
- Modeling the Tertiary Structure of the Rift Valley Fever Virus L-protein. *Molecules 24*, 1768 (2019).
- Polypyrrole on Graphene: A Density Functional Theory Study. *Surface Science* 674, 1 (2018).

Research Focus

My research focuses on the discovery, interpretation, prediction, modeling, simulation, and organization of the microscopic interactions between atoms and molecules in condensed phases of matter and beyond. My research emphasizes the development of the next generation of atomistic and quantum models for simulation of matter, including bio-materials, soft and hard materials. The ability to predict properties of matter is a fundamental requirement of technological advances and economic competitiveness.

Current Projects

- Insights of the solvent effect on a variety of solvated polymers through explicit modeling of the solvent and atomistic modeling of the polymers.
- Discovery of the thermodynamics-structure relations in binary metal alloys, their heat of transformation along phase t ransitions.
- Development of a variety of force fields for macromolecular systems including polymers.
- Structural fingerprints of biomolecules through Molecular Dynamics and Machine Learning approaches.
- Interfacial phenomena between different polymers.