

Department of Physics & Astronomy

Dr. Pengyu Ren

Associate Professor

Department of Biomedical Engineering

The University of Texas at Austin

Friday, February 1, 2013

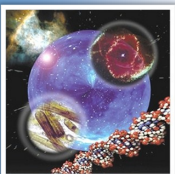
3:00 p.m. - 4:00 p.m.

UC 2.02.02

Modeling Intermolecular Forces in Biomolecules

My lab is interested in understanding the physical forces that are responsible for biomolecular structures and their specific recognition, which are essential to the functions of biomolecules and to the development of molecular diagnostics and therapeutics. I will present a classical model that describes the interatomic electrostatic interactions by means of polarizable atomic multipole moments. Development and application of this model will be demonstrated on small organic molecules and protein-ligand binding. Our ultimate goal is to achieve chemically accurate prediction of biomolecular structure and thermodynamics of molecular interactions. While the results obtained so far are very promising, I will also discuss the challenges ahead and potential improvements we are currently working on.

.



Department Contact Information

Dr. Marcelo Marucho • 210.458.7862 • Marcelo.Marucho@utsa.edu

Nakia Scott • 210.458.5698 • Nakia.Scott@utsa.edu

<http://physics.utsa.edu/>