



Short Curriculum Vitae: Georgios Boulougouris

Current Position: Assistant Professor, Molecular Biology and Genetics, DUTH, Greece

Undergraduate Education: Chemical Engineering NTUA , Greece

Post-graduate Education: NTUA Greece, NCSR “Demokritos” Greece, AMOLF Netherlands

Areas of Interest

- Statistical Mechanics, Thermodynamics, Computational Physical Chemistry, Molecular Simulation, Statistics, Information Theory, Shannon algebra in genetics, computational modeling of biochemical processes .

Distinctions

- Marie Curie Reintegration Grand, Marie Curie individual Fellowship, , NCSR “Demokritos” PhD Fellowship.

Funding

- Host on an [Greek Diaspora Fellowship Program](#), a grant from the Stavros Niarchos Foundation (SNF)

Representative publications

G. C. Boulougouris “Free Energy Calculations, Enhanced by a Gaussian Ansatz, for the “Chemical Work” Distribution”, *Journal of Computational Chemistry*, 2014, 35

G. C. Boulougouris, “Multidimensional direct free energy perturbation”, *J. Chem. Phys.*, 2013, 138, 114111

G.C. Boulougouris, “On the Estimation of the Free Energy, From a Single Equilibrium Statistical Ensemble, via Particle Reinsertion” *J. Phys. Chem. B*, 2012, 116, 997

G. C. Boulougouris, “Calculation of the chemical potential beyond the first order free energy perturbation: from deletion to reinsertion.”, *Journal of Chemical & Engineering Data* , 2010, 6, 1307-1322 (2010)

G. C. Boulougouris, D.N. Theodorou. “Probing sub-glass relaxation in polymers via a geometric representation of probabilities, observables and relaxation modes for discrete stochastic systems.”, *J.Chem.Phys*, **2009**, 130, 044905

G. C. Boulougouris and D.N. Theodorou, ”Dynamical integration of a Markovian web: A first passage time approach” *J.Chem.Phys*, **2007**, 127, 084903

G. C. Boulougouris, D. Frenkel, “Monte Carlo sampling of a Markov web”, *J. Chem. Theory Comput.* **2005**, 1, 389-393

G.C. Boulougouris, I.G. Economou and D.N. Theodorou, " On the Calculation of the Chemical Potential Using the Particle Deletion Scheme ", *Mol. Phys.*, **1999**, 96, 905-913

N. Lempesis, D. Tsalikis G. C. Boulougouris, D.N. Theodorou, "Lumping analysis for the prediction of long-time dynamics: from monomolecular reaction systems to inherent structure dynamics of glassy materials" *J.Chem.Phys*, 2011, 135 pp. 204507.

G.C Boulougouris., I.G Economou. and D.N Theodorou., "Engineering a Molecular Model for Water Phase Equilibrium over a Wide Temperature and Pressure Range", *J. Phys. Chem. B*, **1998**, 102, 1029-1035
