

# POSSIM – Polarizable Simulations with Second order Interaction Model

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POSSIM is a software suite for geometry optimizations and Monte Carlo simulations with fixed-charges (OPLS-like) and polarizable (fast polarizable POSSIM and full-scale polarizable) force fields.

## Selected References for the POSSIM Software:

- (1) Kaminski, G. A.; Ponomarev, S. Y.; Lin, A. B. "Polarizable Simulations with Second-Order Interaction Model – Force Field and Software for Fast Polarizable Calculations: Parameters for Small Model Systems and Free Energy Calculations", *J. Chem. Theory Comput.*, 5, 2935-2943, **2009**.
- (2) Ponomarev, S. Y.; Kaminski, G. A. "Polarizable Simulations with Second-Order Interaction Model (POSSIM) Force Field: Developing Parameters for Alanine Peptides and Protein Backbone", *J. Chem. Theory Comput.*, 7, 1415-1427, **2011**.
- (3) For simulations with Fuzzy-Border continuum solvent model – Sharma, I.; Kaminski, G. A. "Calculating pKa Values for Substituted Phenols and Hydration Energies for Other Compounds with the First-Order Fuzzy-Border Continuum Solvation Model", *J. Comput. Chem.*, 33, 2388-2399, **2012**.

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Dr. George A. Kaminski  
Department of Chemistry and Biochemistry, GP4019  
Worcester Polytechnic Institute  
100 Institute Rd  
Worcester, MA 01609 U.S.A.

A scanned signed copy can also be e-mailed to:  
gkaminski@wpi.edu